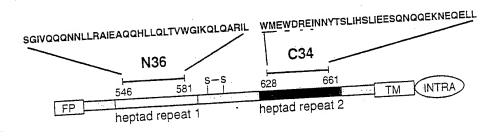
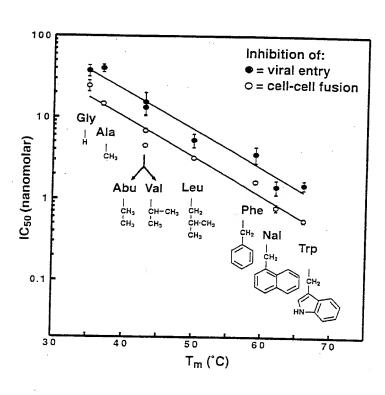
Figure 1: HIV-1 gp41 Structure and Peptides



Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion Inventors:

Debra M. Eckert, et al.

Figure 2: Correlation of C34 Inhibitory Potency With N36/C34 Stability



Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion

Debra M. Eckert, et al.



Figure 3: D-peptide Sequences

Ac-GACEARHREWAWLCAA-CONH2 D10pep1 :

Ac - KK G A C E A R H R E W A W L C A A - CONH2 D10pep1a:

Ac - KK G A C G L G Q E E W F W L C A A - CONH2 D10pep3 :

Ac - GACDLKAKEWFWLCAA - CONH2 D10pep4 :

D10pep5: Ac - KK GACELLGWEWAWLCAA - CONH2 D10pep5a: Ac - KKKK G A C E L L G W E W A W L C A A - CONH2

Ac - G A C S R S Q P E W E W L C A A - CONH2 D10pep6a: Ac - KK G A C S R S Q P E W E W L C A A - CONH2

Ac - KK G A C L L R A P E W G W L C A A - CONH2 D10pep7a:

D10pep10: Ac - KK G A C M R G E W E W S W L C A A - CONH2

D10pep12: Ac - K K G A C P P L N K E W A W L C A A - CONH2

CXXXXXEWXWLC Consensus Sequence

Where:

G = glycine

A = alanine

C = cysteine

D = aspartic acid

L = leucine

K = lysine

E = glutamic acid

W = tryptophan

F = phenylalanine

R = arginine

H = histidine

S = serine

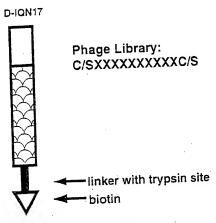
Q = glutamine

Docket/App No.. 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion

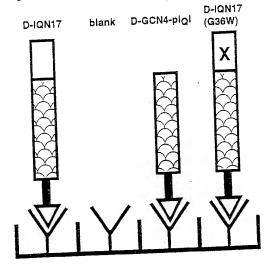
Debra M. Eckert, et al. Inventors:

Figure 4: Mirror-Image Phage Display with the D-IQN17 Target

1. Perform rounds of phage selection to identify binders to D-IQN17.

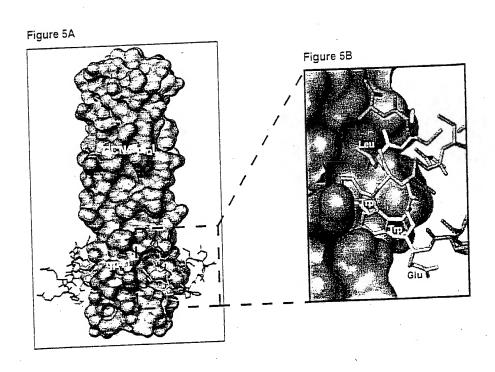


- 2. Sequence individual phage clones
- 3. Test for specificity of binding. Determine if the phage bind to the gp41 region of D-IQN17.



- 4. Synthesize D-peptides.
- 5. Assay anti-HIV activity of D-peptides.

Relationship of D-peptides to IQN17



Syncytia Assays

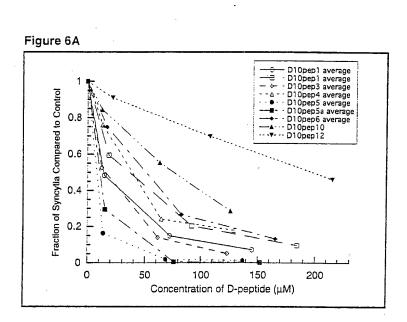


Figure 6B: IC₅₀ Data for D-Peptides:

D-Peptide	Approximate IC ₅₀ Value (from one or more experiments)
D10pep1 D10pep1A D10pep3 D10pep4 D10pep5 D10pep5a D10pep6 D10pep7a	2 x 10 ⁻⁵ M 3 x 10 ⁻⁵ M 1 x 10 ⁻⁵ M 3 x 10 ⁻⁶ M 6 x 10 ⁻⁶ M 3 x 10 ⁻⁵ M 4 x 10 ⁻⁵ M
Dpep10 Dpep12	6 x 10 ⁻⁵ M 2 x 10 ⁻⁴ M

D10pep3 D10pep4 show anti-viral effects with IC₅₀ values of D10pep5 less than 1 x 10⁻⁴ M.



```
REMARK
           REFINEMENT.
REMARK
                           : CNS 0.5
             PROGRAM
                           : BRUNGER, ADAMS, CLORE, DELANO,
REMARK
                             GROS, GROSSE-KUNSTLEVE, JIANG,
              AUTHORS
REMARK
                             KUSZEWSKI, NILGES, PANNU, READ,
REMARK
                             RICE, SIMONSON, WARREN
REMARK
REMARK
          3
REMARK
             DATA USED IN REFINEMENT.
              RESOLUTION RANGE HIGH (ANGSTROMS) : 1,50
REMARK
              RESOLUTION RANGE LOW (ANGSTROMS) :10.00
REMARK
                                       (SIGMA(F)) : 0.0
REMARK
              DATA CUTOFF
                                                       646169.44
                                         (ABS(F)) :
REMARK
              DATA CUTOFF HIGH
                                                        0.000000
                                         (ABS(F)) :
REMARK
              DATA CUTOFF LOW
              COMPLETENESS (WORKING+TEST) (%): 94.6
REMARK
                                                   : 13549
REMARK
              NUMBER OF REFLECTIONS
 REMARK
              FIT TO DATA USED IN REFINEMENT.
 REMARK
                                                  : THROUGHOUT
               CROSS-VALIDATION METHOD
 REMARK
               FREE R VALUE TEST SET SELECTION : RANDOM
 REMARK
                                (WORKING SET) : 0.214
 REMARK
               R VALUE
                                                  : 0.245
 REMARK
               FREE R VALUE
               FREE R VALUE TEST SET SIZE
FREE R VALUE TEST SET COUNT
                                              (%) : .10.1
 REMARK
                                                  : 1362
 REMARK
               ESTIMATED ERROR OF FREE R VALUE : 0.007
 REMARK
 REMARK
              FIT IN THE HIGHEST RESOLUTION BIN.
 REMARK
               TOTAL NUMBER OF BINS USED
 REMARK
                                                  (A) : 1.50
 REMARK
                BIN RESOLUTION RANGE HIGH
                                                  (A): 1.59
 REMARK
                BIN RESOLUTION RANGE LOW
                BIN COMPLETENESS (WORKING+TEST) (%) : 96.1
  REMARK
                                       (WORKING SET) : 2008
  REMARK
                REFLECTIONS IN BIN
                                       (WORKING SET) : 0.233
  REMARK
                BIN R VALUE
                                                      : 0.270
  REMARK
                BIN FREE R VALUE
                BIN FREE R VALUE TEST SET SIZE (%): 9.8
BIN FREE R VALUE TEST SET COUNT : 219
  REMARK
  REMARK
            3
                ESTIMATED ERROR OF BIN FREE R VALUE : 0.018
            3
  REMARK
  REMARK
            3
               NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
  REMARK
  REMARK
                                                0
                                           :
                PROTEIN ATOMS
  REMARK
                                                 0
                NUCLEIC ACID ATOMS
  REMARK
                                                 0
                 HETEROGEN ATOMS
  REMARK
                 SOLVENT ATOMS
  REMARK
   REMARK
               B VALUES.
                                             (A**2) : 21.5
   REMARK
                 FROM WILSON PLOT
                                    (OVERALL, A**2) : 29.7
   REMARK
                 MEAN B VALUE
                 OVERALL ANISOTROPIC B VALUE.
   REMARK
   REMARK
                  B11 (A**2): 3.61
B22 (A**2): 3.61
B33 (A**2): -7.22
   REMARK
   REMARK
   REMARK
                  B12 (A**2) : 1.74
B13 (A**2) : 0.00
   REMARK
   REMARK
                   B23 (A**2) : 0.00
   REMARK
    REMARK
                 BULK SOLVENT MCDELING.
    REMARK
                  METHOD USED : FLAT MODEL
    REMARK
                              : 0.394054
                  KSOL
    REMARK
```

Figure 7A

```
: 58.3445 (A**2)
          BSOL
REMARK
REMARK
          ESTIMATED COORDINATE ERROR.
REMARK
                                   (A) : 0.18
          ESD FROM LUZZATI PLOT
REMARK
                                   (A): 0.09
          ESD FROM SIGMAA
REMARK
                                   (A) : 5.00
          LOW RESOLUTION CUTOFF
REMARK
REMARK
          CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK
                                   (A) : 0.20
          ESD FROM C-V LUZZATI PLOT
REMARK
                                    (A) : 0.12
           ESD FROM C-V SIGMAA
REMARK
REMARK
          RMS DEVIATIONS FROM IDEAL VALUES.
       3
REMARK
                                   (A) : 0.012
           BOND LENGTHS
REMARK
                               (DEGREES) : 1.5
           BOND ANGLES
REMARK
                               (DEGREES) : 15.7
           DIHEDRAL ANGLES
REMARK
                               (DEGREES) : 1.00
           IMPROPER ANGLES
REMARK
REMARK
          ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK
REMARK
                                             RMS
          ISOTROPIC THERMAL FACTOR RESTRAINTS.
REMARK
                                    (A**2) : 0.956
           MAIN-CHAIN BOND
REMARK
                                                 ; 3.0
                                    (A**2) : 1.503
           MAIN-CHAIN ANGLE
REMARK
                                    (A**2) : 1.853
                                                 ; 3.0
           SIDE-CHAIN BOND
REMARK
                                                 ; 3.5
                                    (A**2) : 2.676
           SIDE-CHAIN ANGLE
REMARK
REMARK
          NCS MODEL : NONE
REMARK
 REMARK
                                                 SIGMA/WEIGHT
                                            RMS
          NCS RESTRAINTS.
        3
                                                ; NULL
REMARK
                                       (A) : NULL
           GROUP 1 POSITIONAL
GROUP 1 B-FACTOR
 REMARK
                                    (A**2) : NULL
REMARK
 REMARK
          PARAMETER FILE 1 : protein_rep_d.param
 REMARK
          PARAMETER FILE 2 : CNS_TOPPAR/water_rep.param
 REMARK
           PARAMETER FILE 3 : CNS_TOPPAR/ion.param
 REMARK
           TOPOLOGY FILE 1 : CNS_TOPPAR/protein.top
        3
 REMARK
                           : CNS_TOPPAR/water.top
           TOPOLOGY FILE
                       2
        3
 REMARK
                          : CNS_TOPPAR/ion.top
           TOPOLOGY FILE
        3
 REMARK
 REMARK
          OTHER REFINEMENT REMARKS: NULL
                ACE ARG MET LYS GLN ILE GLU ASP LYS ILE GLU GLU ILE
 REMARK
                 GLU SER LYS GLN LYS LYS ILE GLU ASN GLU ILE ALA ARG
        1 A 214
 SEORES
                 ILE LYS LYS LEU LEU GLN LEU THR VAL TRP GLY ILE LYS
 SECRES
        2 A
            214
                 GLN LEU GLN ALA ARG ILE LEU ACE DLY DLA DCS DLU DLA
        3 A
            214
 SECRES
                 DRG DIS DRG DLU DRP DLA DRP DEU DCS DLA DLA CL WAT
        4 A
             214
 SECRES
                 5 A
             214
 SEORES
                 TAW TAW TAW TAW TAW TAW TAW TAW TAW TAW
         6 A
             214
 SEORES
                 214
         7 A
 SEORES
                 TAW TAW TAW TAW TAW TAW TAW TAW TAW TAW
             214
         8 A
 SECRES
                 WAT WAT WAT TAW TAW TAW TAW TAW TAW TAW
         9 A
             214
 SEQRES
                 214
 SEQRES
        10 A
                 TAW TAW TAW TAW TAW TAW TAW TAW TAW TAW
        11 A
            214
 SEORES
                 12 A
             214
  SEQRES
                 214
        13 A
  SEQRES
                 214
  SEQRES
        14 A
        15 A 214
                 SEORES
        16 A 214
  SEQRES
            214 WAT WAT WAT WAT WAT
         41.829 41.829 84.817 90.00 90.00 120.00 P 3 2 1
        17 A
  SEORES
  CRYST1
                                          0.00000
           1.000000 0.000000 0.000000
  ORIGX1
```

Figure 7B

		0.0000	
ORIGK2	0.000000 1.000000	0.000000 0.00000 3.000000 0.00000	
OP.IGX3	0.000000 0.000000	2.00000	
SCALE1	0.023907 0.013803		
SCALE2	0.000000 0.027605	0.000000	
SCALE3	0.000000 0.000000	0.0==,50	A
ATOM	1 CA ACE A 0	20.330	A
MOTA	2 C ACE A 0	20.773	A
ATOM	3 O ACE A 0	25.055 5.025 25.25	A
ATOM	4 N ARGA 1	27.743	A
ATOM	5 CA ARG A 1	27.023 20.000 1 00 54 54	A
ATOM	6 CB ARG A 1	27.025 11.500 10.00 1 00 54 10	A
ATOM	7 CG ARGA 1	27.041 12.150 20.54 10	A
ATOM	8 CD ARG A 1	27.037 14.003 20.000 2 20 74 00	A
MOTA	9 NE ARGA 1	20.21	A
ATOM	10 CZ ARG A 1	25.270	A
ATOM	11 NH1 ARG A 1	30.333 14.034 20.00 10 77	A
ATOM	12 NH2 ARG A 1	25.045 25.05.	A
ATOM	13 C ARG A 1	20.722 10.007 12.004 1 00 54 51	A
ATOM	14 0 ARG A 1	27.042 10.221 10.00 1 00 54 42	A
ATOM	15 N MET A 2	25,510 5,605 25,405 - 00 54 44	A
ATOM	16 CA MET A 2	24.443 3.072 27.00	A
MOTA	17 CB MET A 2	23.074 3.175	. A
ATOM	18 CG MET A 2	22.745 0.750 20.750 2 00 55 53	A
ATOM	19 SD MET A 2	21,343 3,234 22,20	A
ATOM	20 CE MET A 2	22.100	A
ATOM	21 C MET A 2	24.337 0.300 200 1.00 54.42	A
ATOM	22 O MET A 2	24.075	A
ATOM	23 N LY5 A 3	15.20	A
ATOM:	24 CA LYS A 3	20.000 0.000 0.00 0.00 74 05	A
ATOM	25 CB LYS A 3	20.222 5.255 20.25 2.00 54.04	A
ATOM	26 CG LYS A 3	20.327	A
ATOM	27 CD LYS A 3	27.727	A
ATOM	28 CE LYS A. 3	20.200	A
ATOM	29 NZ LYS A 3	29.332	A
ATOM	30 C LYS A 3	20.037	A
ATOM	31 O LYS A 3	23.775 5.710 50.52 1 00 53 04	A
ATOM	32 N GLNA 4	27.004 7.235 25.50	A
ATOM	33 CA GLN A 4	27.012 1.020 1 00 54 31	A
MOTA	34 CB GLNA 4	20.043	A
ATOM	35 CG GLN A 4	23.002 0.00 0.00 EE EE	A
ATOM	36 CD GLNA 4	23.021 10.200 10.10 1 00 55 10	A
ATOM	37 OE1 GLN A 4	25.555	A
ATOM	38 NE2 GLN A 4	29.555 20.207	A
ATOM	39 C GLN A 4	20.020	A
ATOM	40 0 GLN A 4	20.2.2	A
ATOM	41 N ILE A 5	23.632 6.326 22.70	A
MOTA	42 CA ILE A 5	24.01/	A
MOTA	43 CB ILE A 5	23.820 10.500 11.00 1 00 51 41	A
ATOM	44 CG2 ILE A 5	22.043 10.022 20.04	A
ATOM	45 CG1 ILE A 5	24.34/ 11.021 10.00 1 00 51 73	A
ATOM	46 CD1 ILE A 5	23.010	A
ATOM	47 C ILE A 5	24.001 0.00 1 00 F1 00	A
ATOM	48 O ILE A 5	23.030 0.700 En con a no co en en	A
MOTA	49 N GLUA 6	23.304 7.504 1.00 50 01	A
MOTA	50 CA GLUA 6	23.230	A
ATOM	51 CB GLUA 6	22.705 5.225 and 1 00 st 26	A
MOTA	52 CG GLU A ··· 6	44.141	A
MOTA	53 CD GLUA 6	22.045 4.703 -16.400 1.00 51.68	

Figure 7C

ATOM 54 OEI GLU A 6 23.016 3.931 -16.557 1.00 52.29 ATOM 55 OEZ GLU A 6 21.019 4.682 -17.116 1.00 52.25 AROM 56 C GLU A 6 23.995 5.606 -11.904 1.00 49.32 AROM 57 O GLU A 6 23.475 5.210 -10.859 1.00 49.32 AROM 57 O GLU A 6 23.475 5.210 -10.859 1.00 49.32 AROM 59 CA ASP A 7 25.302 5.527 -12.128 1.00 48.32 AROM 59 CA ASP A 7 25.302 5.527 -12.128 1.00 48.32 AROM 60 CB ASP A 7 27.543 4.626 -11.703 1.00 47.92 AROM 61 CG ASP A 7 27.543 4.626 -11.703 1.00 47.92 AROM 61 CG ASP A 7 27.450 3.585 -12.788 1.00 48.33 AROM 62 OD1 ASP A 7 26.526 2.741 -12.729 1.00 48.43 AROM 63 OD2 ASP A 7 26.324 5.920 -9.926 1.00 48.43 AROM 64 C ASP A 7 26.344 5.920 -9.926 1.00 46.99 AROM 66 N LYS A 8 26.551 7.209 -10.201 1.00 44.57 AROM 66 N LYS A 8 26.551 7.209 -10.201 1.00 44.57 AROM 66 N LYS A 8 26.551 7.209 -10.201 1.00 44.57 AROM 67 CA LYS A 8 26.555 17.209 -10.201 1.00 44.57 AROM 68 CB LYS A 8 26.555 17.209 -10.695 1.00 43.49 AROM 69 CG LYS A 8 26.595 9.598 -9.708 1.00 43.49 AROM 70 CD LYS A 8 26.698 12.490 -11.069 1.00 43.49 AROM 71 CE LYS A 8 26.698 12.490 -11.069 1.00 45.54 AROM 72 NZ LYS A 8 27.153 13.499 -12.069 1.00 45.54 AROM 73 C LYS A 8 27.153 13.499 -12.069 1.00 45.55 AROM 73 C LYS A 8 25.419 8.346 -7.098 1.00 41.55 AROM 75 N ILE A 9 23.015 7.859 -9.335 1.00 41.20 AROM 76 CA ILE A 9 23.015 7.859 -9.335 1.00 41.20 AROM 76 CA ILE A 9 23.015 7.859 -9.358 1.00 37.14 AROM 78 CGZ ILE A 9 21.631 9.303 -9.812 1.00 37.14 AROM 78 CGZ ILE A 9 21.631 9.303 -9.812 1.00 37.14 AROM 80 CDI ILE A 9 22.927 7.653 -7.879 1.00 33.04 AROM 79 CGI ILE A 9 22.927 7.653 -7.879 1.00 33.04 AROM 80 CDI ILE A 9 22.927 7.653 -7.879 1.00 33.04 AROM 80 CDI ILE A 9 22.927 7.653 -7.871 1.00 33.04 AROM 80 CDI ILE A 9 22.927 7.653 -7.879 1.00 33.04 AROM 80 CDI ILE A 9 22.927 7.859 -9.335 1.00 37.29 1.00 33.04 AROM 80 CDI ILE A 9 22.927 7.653 -7.879 1.00 33.04 AROM 80 CDI ILE A 9 22.927 7.653 -7.879 1.00 33.04 AROM 90 C GLU A 10 24.287 0.417 -7.747 1.00 33.56 AROM 90 C GLU A 10 24.287 0.417 -7.747 1.00 33.04 AROM 90 C GLU A 11 25.556 6.377 -2.758 1.00 33.08 AROM	
AROM 56 C GLU A 6 23.995 5.606 -11.904 1.00 49.32 AROM 57 O GLU A 6 23.475 5.210 -10.859 1.00 49.24 AROM 58 N ASP A 7 25.302 5.527 -12.128 1.00 48.32 AROM 59 CA ASP A 7 26.178 4.970 -11.113 1.00 47.23 AROM 60 CB ASP A 7 26.178 4.970 -11.113 1.00 47.92 AROM 61 CG ASP A 7 27.543 4.626 -11.703 1.00 48.33 AROM 62 OD1 ASP A 7 27.543 3.585 -12.788 1.00 48.33 AROM 62 OD1 ASP A 7 26.526 2.741 -12.729 1.00 48.43 AROM 63 OD2 ASP A 7 28.310 3.606 -13.690 1.00 48.94 AROM 63 OD2 ASP A 7 28.310 3.606 -13.690 1.00 48.94 AROM 64 C ASP A 7 26.344 5.920 -9.926 1.00 46.09 AROM 65 O ASP A 7 26.383 5.481 -8.773 1.00 45.71 AROM 66 N LYS A 8 26.551 7.209 -10.201 1.00 44.57 AROM 68 CB LYS A 8 26.551 7.209 -10.201 1.00 44.57 AROM 68 CB LYS A 8 26.959 9.598 -9.708 1.00 43.49 AROM 69 CG LYS A 8 25.895 10.076 -10.695 1.00 44.78 AROM 69 CG LYS A 8 25.895 10.076 -10.695 1.00 45.64 AROM 70 CD LYS A 8 26.698 12.490 -11.068 1.00 45.64 AROM 71 CE LYS A 8 26.698 12.490 -11.006 1.00 45.55 AROM 72 NZ LYS A 8 27.153 13.499 -12.069 1.00 45.55 AROM 73 C LYS A 8 25.419 8.346 -7.098 1.00 43.99 AROM 74 O LYS A 8 25.419 8.346 -7.098 1.00 43.99 AROM 75 N ILE A 9 24.302 7.9355 -9.002 1.00 39.40 AROM 76 CA ILE A 9 22.3015 7.859 -9.358 1.00 37.29 AROM 76 CA ILE A 9 22.3015 7.859 -9.358 1.00 37.14 AROM 78 CGZ ILE A 9 20.600 7.251 -8.759 1.00 37.06 AROM 79 CGI ILE A 9 22.927 6.638 -7.481 1.00 36.07 AROM 79 CGI ILE A 9 22.927 6.638 -7.481 1.00 36.07 AROM 79 CGI ILE A 9 22.927 6.638 -7.481 1.00 33.04 AROM 79 CGI ILE A 9 22.927 6.638 -7.481 1.00 33.04 AROM 79 CGI ILE A 9 22.927 6.638 -7.481 1.00 33.04 AROM 79 CGI ILE A 9 22.927 6.638 -7.481 1.00 33.04 AROM 80 CDI ILE A 9 22.927 6.638 -7.481 1.00 33.04 AROM 80 CDI ILE A 9 22.927 6.638 -7.481 1.00 33.04 AROM 80 CDI ILE A 9 22.927 6.638 -7.481 1.00 33.04 AROM 80 CDI ILE A 9 22.927 6.638 -7.481 1.00 33.04 AROM 80 CDI ILE A 9 22.927 6.638 -7.481 1.00 33.04 AROM 90 C GUU A 10 24.287 0.447 -7.777 1.00 33.56 AROM 90 C GUU A 10 24.287 0.447 -7.777 1.00 33.18 AROM 90 C GUU A 11 25.556 6.337 -7.887 1.00 32.14 AROM 90 C GUU	A
AROM 57 O GLU A 6 23.475 5.210 -10.859 1.00 49.24 AROM 58 N ASP A 7 25.302 5.527 -12.128 1.00 48.32 AROM 59 CA ASP A 7 25.302 5.527 -12.128 1.00 48.32 AROM 69 CB ASP A 7 27.543 4.626 -11.703 1.00 47.23 AROM 60 CB ASP A 7 27.543 4.626 -11.703 1.00 47.23 AROM 61 CG ASP A 7 27.543 4.626 -11.703 1.00 47.23 AROM 62 ODI ASP A 7 26.526 2.741 -12.729 1.00 48.43 AROM 63 OD2 ASP A 7 28.310 3.606 -13.690 1.00 48.94 AROM 64 C ASP A 7 26.526 2.741 -12.729 1.00 48.09 48.00 48.0	A
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ATOM 100 O GLU A 11 25.556 6.377 -2.798 1.00 28.89 ATOM 101 N ILE A 12 24.737 7.640 -4.471 1.00 29.09 ATOM 102 CA ILE A 12 24.017 8.533 -3.550 1.00 28.34 ATOM 103 CB ILE A 12 23.301 9.675 -4.325 1.00 28.74 ATOM 104 CG2 ILE A 12 22.206 10.281 -3.501 1.00 28.70 ATOM 105 CG1 ILE A 12 24.327 10.743 -4.701 1.00 28.84 ATOM 106 CD1 ILE A 12 23.922 11.603 -5.890 1.00 29.69 ATOM 107 C ILE A 12 22.985 7.725 -2.761 1.00 29.69 ATOM 108 O ILE A 12 22.802 7.948 -1.560 1.00 26.46 ATOM 109 N GLU A 13 22.312 6.790 -3.423 1.00 27.40	A
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ATOM 102 CA ILE A 12 24.017 8.533 -3.550 1.00 28.34 ATOM 103 CB ILE A 12 23.301 9.675 -4.325 1.00 28.74 ATOM 104 CG2 ILE A 12 22.206 10.281 -3.501 1.00 28.70 ATOM 105 CG1 ILE A 12 24.327 10.743 -4.701 1.00 28.84 ATOM 106 CD1 ILE A 12 23.922 11.603 -5.890 1.00 29.69 ATOM 107 C ILE A 12 22.802 7.745 -2.761 1.00 29.69 ATOM 108 O ILE A 12 22.802 7.948 -1.560 1.00 26.46 ATOM 109 N GLU A 13 22.312 6.790 -3.423 1.00 27.40	A
ATOM 103 CB ILE A 12 23.301 9.675 -4.325 1.00 28.74 ATOM 104 CG2 ILE A 12 22.206 10.281 -3.501 1.00 28.70 ATOM 105 CG1 ILE A 12 24.327 10.743 -4.701 1.00 28.84 ATOM 106 CD1 ILE A 12 23.922 11.603 -5.890 1.00 29.69 ATOM 107 C ILE A 12 22.985 7.725 -2.761 1.00 27.83 ATOM 108 O ILE A 12 22.802 7.948 -1.560 1.00 26.46 ATOM 109 N GLU A 13 22.312 6.790 -3.423 1.00 27.40	A
ATOM 104 CG2 ILE A 12 22.206 10.281 -3.501 1.00 28.70 ATOM 105 CG1 ILE A 12 24.327 10.743 -4.701 1.00 28.84 ATOM 106 CD1 ILE A 12 23.922 11.603 -5.890 1.00 29.69 ATOM 107 C ILE A 12 22.985 7.725 -2.761 1.00 27.83 ATOM 108 O ILE A 12 22.802 7.948 -1.560 1.00 26.46 ATOM 109 N GLU A 13 22.312 6.790 -3.423 1.00 27.40	A
ATOM 105 CG1 ILE A 12 24.327 10.743 -4.701 1.00 28.84 ATOM 106 CD1 ILE A 12 23.922 11.603 -5.890 1.00 29.69 ATOM 107 C ILE A 12 22.985 7.725 -2.761 1.00 27.83 ATOM 108 O ILE A 12 22.802 7.948 -1.560 1.00 26.46 ATOM 109 N GLU A 13 22.312 6.790 -3.423 1.00 27.40	A
ATOM 106 CD1 ILE A 12 23.922 11.603 -5.890 1.00 29.69 ATOM 107 C ILE A 12 22.985 7.725 -2.761 1.00 27.83 ATOM 108 O ILE A 12 22.802 7.948 -1.560 1.00 26.46 ATOM 109 N GLU A 13 22.312 6.790 -3.423 1.00 27.40	A A
ATOM 107 C ILE A 12 22.985 7.725 -2.761 1.00 27.83 ATOM 108 O ILE A 12 22.802 7.948 -1.560 1.00 26.46 ATOM 109 N GLU A 13 22.312 6.790 -3.423 1.00 27.40	
ATOM 108 0 ILE A 12 22.802 7.948 -1.560 1.00 26.46 ATOM 109 N GLU A 13 22.312 6.790 -3.423 1.00 27.40	A
ATOM 109 N GLU A 13 22.312 6.790 -3.423 1.00 27.40	A A
	A A
amov 110 da diti a 12 - 71 313 - 5 965 -7 767 1 00 76 57	A A
ATOM 110 CA GLU A 13 21.313 5.965 -2.762 1.00 26.92 arom 131 CB GLU A 13 20.579 5.087 -3.805 1.00 28.34	A A
ATOM 111 CB GLU A 13 20.579 5.087 -3.805 1.00 28.34	м

Figure 7D

		19.760 5.927 -4.810 1.00 29.72 A	
ATOM	112 CG GLU A 13	19.760 5.327 5.900 1.00 31.77 A	
ATOM	113 CD GLU A 13	19.000 3.22 1 00 33 64 A	
	114 OE1 GLU A 13	19.0/1 4.107 5.227 1.00 32.24 A	
MOTA	115 OE2 GLU A 13	17.900 1.100 26.36 A	
atom atom	116 C GLU A 13	21.9/5 3.110 2.75 A	
ATOM	117 O GLU A 13	21.411 1.311 a on 1 on 26 17 A	
	118 N SER A 14	23.179 1.022 -0.099 1.00 26.31 A	
ATOM ATOM	119 CA SER A 14	23.535 3.324 -1.625 1.00 26.71 A	
ATOM	120 CB SER A 14	25.184 3.470 -0.595 1.00 30.07 A	
ATOM	121 OG SER A 14	23.534 0 101 1 00 25 81 A	
ATOM	122 C SER A 14	24.240 A 149 1.339 1.00 25.13 A	
ATOM	123 O SER A 14	24.075 5.840 0.009 1.00 24.70 A	
ATOM	124 N LYS A 15	25 201 6 713 1.151 1.00 25.41	
ATOM	125 CA LYS A 15	25.005 7 971 0.672 1.00 26.20	
ATOM	126 CB LYS A 15	7 762 0.285 1.00 29.07 A	
ATOM	127 CG LYS A 15	27 275 9 077 -0.220 1.00 30.97	
ATOM	128 CD LYS A 15	27.330 8 914 -0.603 1.00 32.08	
ATOM	129 CE LYS A 15	20.547 7.749 -1.502 1.00 34.63	<u>.</u>
ATOM	130 NZ LYS A 15	23 824 7.102 1.938 1.00 24.43	-, -,
ATOM	131 C LYS A 15	23.862 7.279 3.171 1.00 24.30	a. A.
ATOM	132 O LYS A 15	22 708 7.254 1.247 1.00 24.12	A.
ATOM	133 N G227 11	21 450 7.586 1.904 1.00 23.02	A.
MOTA	134 62 521	20 396 7.815 0.834 1.00 43.71	A.
MOTA	133 65 5-1	19.229 8.643 1.232 1.00 29.04	A
ATOM	136 CG CELL 16	18 543 9.230 0.004 1.00 54.25	A
ATOM	137 (1) (22.1.1.	18.015 8.498 -0.81/ 1.00 54.0	A
MOTA	130 022 023 16	18.569 10.556 -0.135 1.00 32.74	A
MOTA	139 NEZ GEZ 1	21.027 6.447 2.838 1.00 23.84	A
MOTA	140 0 0227 1 16	20.584 6.681 3.979 1.00 22.03	A
MOTA	141 0 0221	21.160 5.214 2.363 1.00 22.59	A
MOTA	142 N 222	20.798 4.037 2.257 1.00.22.86	A
ATOM	143 CA LYS A 17	20.939 2.732 3.055 1.00.26.69	A
MOTA	145 CG LYS A 17	20.340 1.555 2.632 1.00.29.27	A
ATOM	146 CD LYS A 17	18.83/ 1.00 31.75	A
ATOM ATOM	147 CE LYS A 17	18.1//	A
ATOM	148 NZ LYS A 17	16.686 0.376 4.406 1.00 22.31	A
ATOM	149 C LYS A 17	21.718 3.747 5.515 1.00 21.02	A
MOTA	150 O LYS A 17	21.201 4.306 4.223 1.00 21.81	A
ATOM	151 N LYS A 18	23.001 4.302 5.374 1.00 21.74	A
ATOM	152 CA LYS A 18	35 348 4.540 4.964 1.00 24.04	A.
ATOM	153 CB LYS A 18	26 029 3.321 4.401 1.00 27.30	A A
ATOM	154 CG LYS A 18	27 381 3,712 3.863 1.00 29.23	A
ATOM	155 CD LYS A 18	27 972 2.592 3.025 1.00 30.50	A.
MOTA	100 CL 240	29.290 3.010 2.4/2 1.00 33.31	A
MOTA	15/ NZ 215 19	23.500 5.376 6.378 1.00 20.32	A
ATOM	150 C 225 10	23.565 5.138 7.577 1.00 15.05	A
MOTA	159 0 225 3 10	23.062 6.331 3.262 1.00.10.08	A
MOTA	160 N 11E A 19	22.655 7.636 5.762 1.00 10.00	A
ATOM	161 CR 222 1	22.406 8.926 5.914 1.00 20.00	A
MOTA	162 CD 11E A 19	21.554	A
ATOM	163 CG2 222 11,	23.756 3.432 4.205 1.00.21.18	A
ATOM	104 CG1 112 1 19	23.669 10.495 7 537 1 00 20.44	A
ATOM	1 100 CD1 117 1 19	21.400	A
ATOM	1 166 C TIF A 19	21.282	A
MOTA	250 N CTILA 20	20.459 6.365 7.503 1.00.20.43	A
ATOM ATOM	1 co co citi a 20	19.230 6.149 7.503. 1.00 20.43	
ATOM	202	Figure 7E	

Figure 7E

		18.223	5.608	6.484	1.00 22.94	A
MOTA	170 CB GLU A 20	17.766	6.671	5.499	1.00 25.51	A
MOTA	171 CG GLU A 20	16.926	6.108	4.378	1.00 29.04	Α
MOTA	172 CD GLU A 20	16.961	4.873	4.177	1.00 30.40	A
MOTA	173 OE1 GLU A 20	16.243	6.901	3.691	1.00 30.73	A
MCTA	174 OE2 GLU A 20	19.533	5.109	8.576	1.00 20.88	A
MOTA	175 C GLU A 20	18.917	5.127	9.545	1.00 20.23	A
ATOM	176 O GLU A 20	20.478	4.220	8.321	1.00 20.53	A
ATOM	177 N ASN A 21	20.470	3.212	9.328	1.00 21.87	A
ATOM	178 CA ASN A 21	21.694	2.117	8.720	1.00 24.15	A
MOTA	179 CB ASN A 21	20.875	1.155	7.872	1.00 25.28	A
ATOM	180 CG ASN A 21	19.676	0.980	8.099	1.00 28.26	A
ATOM	101 002 > 01	21.505	0.549	6.870	1.00 26.78	A
MOTA	102 1102 1101	21.500	3.854	10.527	1.00 21.75	A
MOTA	105 C 1001	21.269	3.444	11.674	1.00 21.80	A
ATOM	104 0 11-11	22.335	4.853	10.274	1.00 20.99	A
MOTA	103 14 424	23,007	5.548	11.369	1.00 20.36	A
ATOM		24.059	6.516	10.825	1.00 22.89	A
MOTA	107 02 020	24.914	7.169	11.901	1.00 25.86	A
ATOM	100 00 000	25.515	6.170	12.882	1.00 27.97	A
MOTA	10) 05 000	26.121	5.158	12.444	1.00 30.05	A
MOTA	190 001 000	25.376	6.411	14.118	1.00 31.29	A
ATOM	191 000 000	21.952	6.294	12.187	1.00 19.79	A A
ATOM	192 C GLU A 22 193 O GLU A 22	21.988	6.264	13.445	1.00 18.87	A
MOTA	195 0 020	21.003	6.951	11.518	1.00 18.92	A
MOTA	194 N ILE A 23	19.955	7.670	12.254	1.00 18.60	A
ATOM	196 CB ILE A 23	19.012	8.388	11.244	1.00 18.79	A
ATOM	197 CG2 ILE A 23	17.672	8.764	11.880	1.00 20.11	A
ATOM	198 CG1 ILE A 23	19.739	9.598	10.701	1.00 20.45 1.00 22.51	A
ATOM	199 CD1 ILE A 23	19.060	10.223	9.539	1.00 19.09	A
MOTA	200 C ILE A 23	19.163	6.687	13.118	1.00 19.09	A
ATOM ATOM	201 O ILE A 23	18.807	7.006	14.260	1.00 18.44	A
ATOM	202 N ALA A 24	18.903	5.479	12.617 13.420	1.00 18.86	A
ATOM	203 CA ALA A 24	18.153	4.517	12,573	1.00 19.39	A
ATOM	204 CB ALA A 24	17.824	3.257	14.665	1.00 18.66	A
ATOM	205 C ALA A 24	18.947	4.136	15.757	1.00 19.32	A
ATOM	206 O ALA A 24	18.343	3.966	14.548	1.00 18.57	· A
ATOM	207 N ARG A 25	20.272	4.028	15.709	1.00 19.19	A
ATOM	208 CA ARG A 25	21.111	3.667	15.287	1.00 20.85	A
ATOM	209 CB ARG A 25	22.552	1.959	14.627	1.00 23.87	A
ATOM	210 CG ARG A 25	22.674	1.536	14.429	1.00 25.32	A
ATOM	211 CD ARG A 25	24.108 24.759	2.294	13.376		A
ATOM	212 NE ARG A 25	24.733	2.019	12.075		A
ATOM	213 CZ ARG A 25	23.955	0.979	11.641		A
ATOM	214 NH1 ARG A 25	25.296	2.806	11.214		A
ATOM	215 NH2 ARG A 25	21.083	4.819	16.722	1.00 18.69	. A
ATOM	216 C ARG A 25	20.942	4.592	17.940	1.00 17.93	A
MOTA	217 O ARG A 25	21.201	6.041	16.221		A
MOTA	210 1 112 11	21.184	7.222	17.080		A
MOTA	219 01	21.369	8.479			A
MOTA	220 02 06	20.943	9.741			A
MOTA	221 002	22.821	8.537	15.796		A
MOTA	222 001 111 1	23.144	9.587	14.72	1.00 21.83	A
MOTA	223 422	19.876	7.301	17.85	7 1.00 18.02	A
ATOM	227	19.875	7.580			A
ATOM	223 0	18.752	7.069			A
MOTA	226 N LYS A 27 227 CA LYS A 27	17.450			3 1.00 17.90	A
A TOM	221 CM DIS A 21	_				

Figure 7F

Docket/App No.. 0399.1192-008
Title: Inhibitors of HIV Membrane Fusion

Debra M. Eckert, et al. Inventors:

									1 00 10 01	*
ATOM	328	CB	LYS	A.	27	16.330	6.994	16.805	1.00 19.01	A
ATOM	229	CG	LYS	A	27	16.266	8.210	15.876	1.00 22.27	A
ATOM	230	CD	LYS		27	15.275	7.984	14.711	1.00 24.03	A
		CE	LYS		27	13.860	7.664	15.161	1.00 24.41	A
ATOM	231				27	13.173	2.848	15.714	1.00 27.04	A
ATOM	232	NZ	LYS					18.969	1.00 18.17	A
ATOM	233	C	LYS	À	27	17.326	6.097		1.00 18.33	A
ATOM	234	O.	LYS	À	27	16.767	6.388	20.013		
ATOM	235	N	LYS	Α	28	17.871	4.896	18.775	1.00 17.00	A
ATOM	236.	CA	LYS	Α	28	17.788	3.867	19.790	1.00 17.21	A
ATOM	237	CB		A	28	18.244	2.503	19.223	1.00 18.92	A
	238	CG		A	28	17.288	1.982	18.164	1.00 24.56	A
ATOM				A	28	17.833	0.732	17.464	1.00 26.88	A
MOTA	239	CD				16.950	0.371	16.260	1.00 28.84	A
MOTA	240	CE	LYS		28		-0.938	15.592	1.00 31.36	A
MOTA	241	NZ	LYS		28	17.284		21.016	1.00 17.36	A
MOTA	242	C	LYS	Α	28	18.618	4.257			
ATOM	243	Ο.	LYS	Α	28	18.169	4.066	22.165	1.00 17.54	A
ATOM	244	N	LEU	Α	29	19.794	4.835	20.793	1.00 16.84	A
ATOM	245	CA	LEU	Α	29	20.642	5.234	21.912	1.00 16.41	A
ATOM	246	CB	LEU		29	22.077	5.529	21.453	1.00 16.26	,Α
	247	CG	LEU		29	23.050	6.048	22.515	1.00 16.76	A
ATOM			LEU		29	23.062	5.096	23.701	1.00 16.47	A
ATOM	248					24.450	6.201	21.885	1.00 17.67	A
ATOM	249		LEU		29			22.606	1.00 16.92	A
ATOM	250.	C		A	29	20.023	6.429		1.00 16.36	A
ATOM	251	0	LEU	Α	29	20.027	6.503	23.859		
ATOM	252	N	LEU	A	30	19.447	7.343	21.820	1.00 15.57	A
ATOM	253	CA	LEU	Α	30	18.818	8.519	22.424	1.00 15.77	A
ATOM	254	CB	LEU	A	30	18.401	9.501	21.298	1.00 15.65	A
ATOM	255	CG	LEU		30	17.717	10.780	21.696	1.00 17.55	A
	256		LEU		30	18.557	11.504	22.722	1.00 16.71	A
ATOM					30	17.552	11.602	20,399	1.00 18.10	A
ATOM	257		LEU			17.659	8.067	23.288	1.00 16.42	A
ATOM	258	С	LEU		30		8.604	24.399	1.00 17.55	A
ATOM	259	0	LEU		30	17.466		22.862	1.00 16.79	A
ATOM	260	N	GLN	A	31	16.903	7.053			A
ATOM	261	CA	GLN	Α	31	15.816	6.564	23.692	1.00 18.13	
ATOM	262	CB	GLN	Α	31	14.945	5.593	22.386	1.00 21.45	A
ATOM	263	CG	GLN	Α	31	14.119	6.358	21.834	1.00 24.92	A
ATOM	264	CD	GLN		31	13.196	7.437	22.424	1.00 26.81	A
ATOM	265		GLN		31	12.913	8.459	21.786	1.00 28.75	A
	266	NE2			31	12.713	7.207	23,648	1.00 29.86	A
MOTA					31	15.319	5.958	25.008	1.00 17.24	A
ATOM	267	С	GLN			15.655	6.092	26.038	1.00 17.79	A
MOTA	268	0	GLN		31		5.307	24.987	1.00 15.77	A
ATOM	269	N	LEU		32	17.494			1.00 14.63	A
ATOM	270	CA	LEU	Α	32	18.070	4.755	26.209		A
ATOM	271	CB	LEU	A	32	19.314	3.932	25.911	1.00 16.13	
ATOM	272	ÇG	LEU	Α	32	19.015	2.574	25.275	1.00 18.58	A
ATOM	273	CD1	LEU	Α	32	20.291	1.961	24.770	1.00 20.70	A
ATOM	274		LEU	Α	32	18.337	1.698	26.315	1.00 22.17	A
	275	C	LEU		32	18.449	5.895	27.140	1.00 13.68	A
ATOM		Ö	LEU		32	18.258	5.774	28.357	1.00 13.31	A
ATOM	276				33	18.980	6.991	26.600	1.00 13.42	A
MOTA	277	N	THR				8.081	27.500	1.00 12.96	A
MOTA	278	CA	THR		33	19.348		26.820	1.00 13.48	A
ATOM	279	CB	THE		33	20.236	9.134			
ATOM	280	OG1	THR	Α	33	19.530	9.745	25.733	1.00 15.60	A
ATOM	281	CG2	THR	Α	33	21.567	8.508	26-358	1.00 15.01	A
ATOM	282	С	THR		33	18.124	8.742	28.117	1.00 13.65	· A
ATOM	283	ō	THR		33	18.159	9.169	29.285	1.00 12.67	A
	284	N	VAL		34	17.038	8.838	27.345	1.00 13.20	A
ATOM		CA	VAL		34	15.804	9.410	27.863	1.00 13.88	A
MOTA	285	C.M.	سد ۷		2-4					

Figure 7G

343 N

ATOM

Docket/App No.: 0399.1192-008 Inhibitors of HIV Membrane Fusion Title:

Debra M. Eckert, et al.

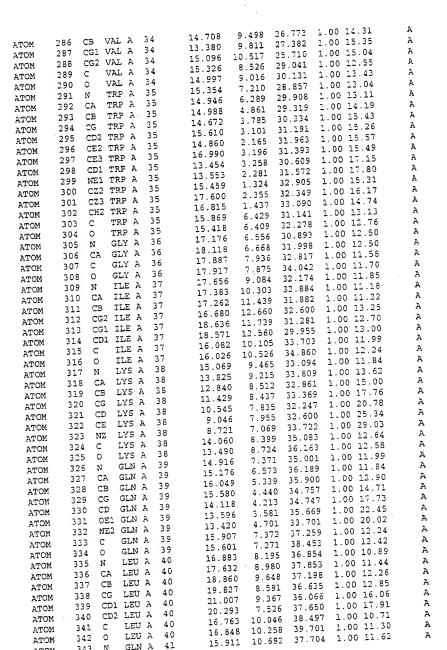


Figure 7H

3 mOM	344	CA	GLN A	41	15.038	11.695	38.322	1.00 11.12	A
ATOM		CB	GLN A	41	14.241	12.447	37.257	1.00 11.92	A
MOTA	345		GLN A	42	13.250	13.381	37.845	1.00 11.53	A
ATOM	346	CG			12.280	13.933	36.838	1.00 12.64	A
MOTA	347	CD	GLN A	41		13.226	35.962	1.00 13.16	A
MOTA	348	OE1	GLN A	41	11.814			1.00 13.67	A
MOTA	349	NE2	GLN A	41	11.972	15.220	36.973		A
ATOM	350	С	GLN A	41	14.081	11.031	39.332	1.00 10.98	
ATOM	351	0	GLN A	41	13.883	11.585	40.404	1.00 12.39	A
ATOM	352	N	ALA A	42	13.571	9.845	38.994	1.00 12.53	À
ATOM	3 5 3	CA	ALA A	42	12.642	9.185	39.928	1.00 12.08	A
ATOM	354	CB	ALA A	42	12.035	7.954	39.295	1.00 13.83	A
	355	C	ALA A	42	13.383	8.856	41.218	1.00 14.57	A
ATOM			ALA A	42	12.820	8.975	42.296	1.00 15.73	A
ATOM	356	0		43	14.647	8.446	41.147	1.00 13.64	A
MOTA	357	N	ARG A		15.412	8.150	42.327	1.00 16.22	A
ATOM	358	CA	ARG A	43		7.626	41.852	1.00 18.06	A
MOTA	359	CB	ARG A	43	16.772			1.00 22.64	A
MOTA	360	CG	ARG A	43	17.706	7.309	42.895		A
ATOM	361	CD	ARG A	43	17.232	6.108	43.679	1.00 25.20	
ATOM	362	NE	ARG A	43	18.302	5.922	44.577	1.00 27.65	A
ATOM	363	CZ	ARG A	43	18.943	4.798	44.758	1.00.20.75	- A
ATOM	364		ARG A	43	18.607	3.666	44.107	1.00 24.75	A
	365		ARG A	43	19.983	4.899	45.516	1.00 23.93	A
ATOM		C	ARG A	43	15.606	9.411	43.196	1.00 15.07	A
ATOM	366		ARG A	43	15.441	9.372	44.435	1.00 17.46	A
MOTA	367	<u>`</u> 0		44	15.930	10.529	42.553	1.00 14.44	A
MOTA	368	N	ILE A		16.181	11.794	43.242	1.00 14.63	A
ATOM	369	CA	ILE A	44		12.854	42.280	1.00 15.70	A
ATOM	370	CB	ILE A	44	16.801		42.941	1.00 16.89	A
ATOM	371		ILE A	44	16.817	14,226		1.00 16.08	A
MOTA	372	CG1	ILE A	44	18.236	12.422	41.940		A
ATOM	373	CD1	ILE A	44	18.765	13.127	40.739	1.00 19.48	
ATOM	374	С	ILE A	44	14.906	12.326	43.887	1.00 16.35	A
ATOM	375	0	ILE A	44	14.984	12.862	44.991	1.00 19.28	A
ATOM	376	N	LEU A	45	13.747	12.150	43.258	1.00 15.72	A
ATOM	377	CA	LEU A	45	12.515	12.682	43.883	1.00 15.80	A
ATOM	378	CB	LEU A	45	11.505	13.032	42.801	1.00 15.66	A
	379	CG	LEU A	45	11.867	14.181	41.378	1.00 15.35	A
MOTA				45	10.793	14.298	40.823.	1.00 17.27	A
MOTA	380	CD1			11.954	15.485	42.701	1.00 18.49	A
ATOM	381	CD2		45	11.903	11.710	44.867	1.00 18.22	A
ATOM	382	C	LEU A	45		12.187	45.658	1.00 19.14	A
ATOM	383	Ο.	LEU A	45	11.053		44.884	1.00 20.39	A
ATOM	384	NT	LEU A	45	12.258	10.488		1.00 41.14	В
MOTA	385	CA	ACE D	0	10.275	-0.794	28.942		3
ATOM	386	C	ACE D	0	11.674	-0.285	28.785	1.00 40.52	3
ATOM	387	0	ACE D	0	11.905	0,677	28.016	1.00 41.12	
ATOM	388	N	DLY D	1	12.631	-0.899	29.487	1.00 39.74	В
ATOM	389	CA	DLY D	1	13.997	-0.423	29.356	1.00 37.31	В
ATOM	390	С	DLY D	1	15.200	-1.051	30.044	1.00 35.38	В
ATOM	391	ō	DLY D	. 1	15.133	-2.044	30.785	1.00 35.49	В.
		N	DLA D	2	16:332	-0.424	29.752	1.00 33.19	В
MOTA	392		DLA D	2	17.639	-0.797	30.279	1.00 31.99	В
ATOM	393	CA		2	18.688	0.196	29.762	1.00 31.34	B
MOTA	394	CB	DLA D			-2.217	29.871	1.00 31.71	3
ATOM	395	С	DLA D		18.026	-2.982	30.647	1.00 31.67	В
ATOM	396	0	DLY D		18.611			1.00 30.76	3
ATOM	397	N	DCS D		17.699	-2.577	28.640	1.00 30.70	3
MOTA	398	CA	DCS D		18.061	-3.892	28.159		3
ATOM	399	С	DCS D		17.104	-4.987	28.618	1.00 31.69	
ATOM	400	0	DCS D	3	17.531	-6.020	29.111	1.00 31.85	3
ATOM	401	CB	DCS D	3	18.128	-3.876	26.638	1.00 30.00	3
7.011									

Figure 71

			E
	402 SG DCS D 3	19.502 -2.991 25.840 1.00 30.98	В
MOTA	403 N DLU D 4	15.813 -4.730 20.034 1 00 32.07	₿
MOTA	404 CA DLU D 4	14.782 -3.702 20.534 1 00 33 43	В
MOTA	405 CB DLU D 4	13.397	В
MOTA	406 CG DLU D 4	13.000 -4.044 26.500 1 00 36 29	B
ATOM	407 CD DLU D 4	13.663 -3.366 37 100 37 11	В
	408 OE1 DLU D 4	14.422 -2.639 27.200 - 0.0 37.45	В
ATOM ATOM	409 OE2 DLU D 4	13.367 -3.204 20 276 1 00 31 86	В
ATOM	410 C DLU D 4	14.875 - 201 20 553 1 00 32.10	В
MOTA	411 O DLU D 4	14.632	В
ATOM	412 N DLA D 5	15.022 3.00 30 61	В
ATOM	413 CA DLA D 5	13.030 1.00 30.83	В
ATOM	414 CB DLA D 5	16 362 -6 340 33.008 1.00 30.19	В
ATOM	415 C DLA D 5	16 387 -7.044 34.027 1.00 30.60	В
ATOM	416 O DLA D 5	12 410 -6 202 32,216 1.00 29.09	В
ATOM	417 N DRG D 6	10 573 -6 893 32.489 1.00 28.71	B B
MOTA	418 CA DRG D 6	10 400 -8 408 32.369 1.00 31.46	В
MOTA	419 CB DRG D 6	18 169 -8.847 30.969 1.00 34.88	В
MOTA	420 00 510 5	19.397 -8.762 30.070 1.00 37.42	В
ATOM	421 05 510 5	19.715 -7.408 29.607 1.00 40.20	В
ATOM	422 NL 580 -	20.121 -7.134 28.370 1.00 40.89	В
MOTA	423 02 200	20.248 -0.220	В
MOTA	424 NIII DAG -	20.409 -5.85= 25.55	В
ATOM	425 NH2 DRG D 6	19.313 20.302 33.43	В
ATOM	427 O DRG D 6	19.994 -7.423 31.1-1	В
MOTA	428 N DIS D 7	19.100 23.373 25 624 1 00 22 04	·B
MOTA	429 CA DIS D 7	19.731 25.010 36.384 1 00 22.68	B
ATOM ATOM	430 CB DIS D 7	18.970 -3.000 36.254 1 00 22.88	В
ATOM	431 CG DIS D 7	17.600 - 567 27 104 1 00 24.08	В
MOTA	432 CD2 DIS D 7	17.1/8 -3.307 37 1 00 25.78	В
ATOM	433 ND1 DIS D 7	15.650 -4.134 37.608 1.00 26.45	В
ATOM	434 CE1 DIS D 7	15.393 -5.419 37.562 1.00 25.11	В
ATOM	435 NE2 DIS D 7	21 156 -4 636 35.329 1.00 21.84	В
ATOM	436 C DIS D 7	22 412 -3 743 34.536 1.00 20.32	B B
ATOM	437 0 222	22 091 -5.298 36.003 1.00 20.33	В
MOTA	430 14 22.0	23.494 -5.122 35.778 1.00 19.80	В
MOTA	433 C.1 2.11	24.284 -5.994 36.755 1.00 26.87	3
ATOM	440 CB DRC D	24.175 -7.428 36.459 1.00 20.57	В
ATOM	441 CG DRG D 8	24.743 -0.207 1.00 21 5/	В
MOTA	443 NE DRG D 8	24.581 29.000 31.94	В
ATOM	444 CZ DRG D 8	25.258 410.103 25 550 3 00 33 88	В
MOTA MOTA	445 NH1 DRG D 8	26.139	В
MOTA	446 NH2 DRG D 8	24.307 -11.132 25 072 1 00 17.95	В
ATOM	447 C DRG D 8	23.985 -3.712 25 124 1 00 17.42	В
ATOM	448 O DRG D 8	24.856 -3.504 26.793 1 00 16.93	В
ATOM	449 N DLUD 9	23.407 2.550 2005 1 00 15.49	В
ATOM	450 CA DLU D 9	23.360 -0.954 38.261 1.00 16.03	В
MOTA	451 CB DLU D 9	23 976 -0 652 38.323 1.00 16.75	В
ATOM	452 CG DLU D	22.000 1 816 38 786 1.00 16.82	В
ATOM	453 CD DLU D 9	20.350 -2 982 38.584 1.00 19.63	В
ATOM	454 OE1 DLU D 9	19.933 -1.498 39.310 1.00 20.12	B B
MOTA	455 OE2 DLU D 9	23.601 -0.717 35.747 1.00 15.97	. в
ATOM	456 C DLU D 3	24 142 0.383 35.655 1.00 15.24	В
ATOM	45/ 0 220 2 10	22.747 -1.186 34.844 1.00 15.00	В
ATOM	מו מו פונו מו מו מו מו	22.462 -0.435 33.611 1.00 15.31	_
ATO	4 459 CA DRP D 10	·	
		Figure 7.I	

Figure 7J

	10	20.960 -0.187 33.420 1.00 16.05	В.
MOTA	460 CE DRP D 10	20 354 0.791 34.410 1.00 15.28	В
ATOM	401 00 000	20 504 2 200 34.384 1.00 15.48	Б
ATOM	462 CD2 DRP D 10	10 734 3.730 35.424 1.00 15.74	3
MOTA	463 CE2 DRP D 10	23 237 3 075 33 563 1.00 15.47	В
ATOM	464 CE3 DRP D 10	19.504 0.512 35.449 1.00 16.40	В
ATOM	465 CD1 DRP D 10	19.122 1.676 36.073 1.00 17.22	В
ATOM	466 NE1 DRP D 10	19.650 4.107 35.666 1.00 15.81	В
ATOM	467 CZ2 DRP D 10	22 20 20 10 14 93	В
ATOM	468 CZ3 DRP D 10	22.27	В
MOTA	469 CH2 DRP D 10	20.302	В
ATOM	470 C DRP D 10	23.000 2.50	В
ATOM	471 O DRP D 10	22.790 =0.002 00.000 1 77 72	В
ATOM	472 N DLA D 11	23.744 2.527 21 407 1 00 18 88	B
ATOM	473 CA DLA D 11	24.253 -2.940 32.057 1 00 20 11	B
ATOM	474 CB DLA D 11	25.034 -4.100 32.501 1 00 18 95	B
ATOM	475 C DLA D 11	25.126 -2.074 00.05 1 00.21 13	В
ATOM	476 O DLA D 11	25.070 -2.222	В
ATOM	477 N DRP D 12	25.884 -1.144 5-1-1 1 00 17 72	В
ATOM	478 CA DRP D 12	26.739 20.273 20.20 1 00 18 43	В
ATOM	479 CB DRP D 12	27.300 0.043 0.00 1.00 16.68	В
ATOM	480 CG DRP D 12	26.725 1.500 52.576 1.00 16:49	В
ATOM	481 CD2 DRP D 12	25.285 2.900 32.704 1 00 15 68	В
ATOM	482 CE2 DRP D 12	25.459 5.572 55 1 00 17 14	B
ATOM	483 CE3 DRP D 12	20.519 3.714 33 355 1 00 15 60	В
ATOM	484 CD1 DRP D 12	20.177 1.333 32 550 1 00 15 74	В
ATOM	485 NE1 DRP D 12	25.402 2.400 32.401 1 00 15 78	В
ATOM	486 CZ2 DRP D 12	24.042 1.020 00 505 11 00 17 42	В
	487 CZ3 DRP D 12	25.904 4.57 22 550 1 00 15 81	В
ATOM	488 CH2 DRP D 12	25.090 5.400 52.100 18 81	В
ATOM	489 C DRP D 12	25.913 0.51 20 221 1 00 20 05	В
ATOM	490 O DRP D 12	26.347 0.070 20 700 1 00 17 43	В
ATOM	491 N DEU D 13	24.740 1.020 1.00 17 59	В
ATOM	492 CA DEU D 13	23.915 1.000 20.000 1 00 15 97	В
ATOM	493 CB DEU D 13	22.003 2.00 00 10 1 1 00 15 31	В
ATOM ATOM	494 CG DEU D 13	41.00/ 3.400 004 1 00 15 00	В
	495 CD1 DEU D 13	22.333	В
ATOM ATOM	496 CD2 DEU D . 13	20.000 4.200 - 047 1 00 19 32	В
	497 C DEU D 13	23.203 1.011 1.00 20 12	В
MOTA	498 O DEU D 13	23.424 1.422 100 1 20 20 93	В
ATOM ATOM	499 N DCS D 14	42.773 -0.120 00 106 7 00 22 79	В
ATOM	500 CA DCS D 14	22.190 -1.040 20.124 1 00 27 54	В
ATOM	501 C DCS D 14	23.2/2 -1.323 24.224 3 00 23 67	В
	502 O DCS D 14	22.903 -2.520 27 074 3 00 23 47	В
MOTA	503 CB DCS D 14	21.6/5 -2.515 20.732 1 00 27 91	В
ATOM	504 SG DCS D 14	21.210 -3.000 20.11-	В
ATOM	505 N DLA D 15	24.514 -1.500 25.514 1 00 23 31	В
ATOM	506 CA DLA D 15	25.627 -1.657 -1.67 1.00 24 09	В
MOTA	507 CB DLA D 15	26.860 -2.502	В
MOTA MOTA	508 C DLA D 15	25.987, -0.072 22.724 1 00 25 93	В
ATOM	509 O DLA D 15	26.511 -0.544 25.022 1.00 22 60	. В
ATOM	510 N DLA D 16	25.723 0.344 23.202 1 00 22 10	В
	511 CA DLA D 16	26.01/ 1./43 21.00 1 00 22 02	В
ATOM	512 CB DLA D 16	26.006 2.303 23.020 1.00 21.95	В
MOTA	513 C DLA D 16	24.993 2.992 20 200 1 00 22 36	В
MOTA	514 O DLA D 16	25.355 2.370 22.350 - 0.00 23.47	3
MOTA	515 NT DLA D 16	23.843 1.400 23.72	Ī
MOTA	22 5 7 1 CT T 1	20.914 12.00	W
MOTA	517 OH2 WAT W 1	23,911 6,454 -21,684 1,00 53,50	••
MOTA	J_1 0	· ·	

Figure 7K

2.444 -19.357 3.971 -17.693 1.00 30.822 OH2 WAT W 1.00 37.33 MOTA 518 13.971 30.369 3 WAT w 1.00 46.63 OH2 519 -16.588 12.875 ATOM 27.699 1.00 48.41 WAT W OH2 520 1.727 -13.168 ATOM 23.417 5 1.00 58.65 OH2 WAT 1.401 -16.007 521 ATOM 24.012 ó OH2 WAT W 1.00 36.12 ATOM 522 3.069 -7.418 16.572 OH2 WAT W 1.00 55.01 523 -8.334 MOTA 11.028 32.381 8 WAT W 1.00 53.14 OH2 MOTA 524 7.275 -10.261 33.753 9 1.00 28:89 W WAT W OH2 ATOM 525 -0.862 -12.067 20.318 WAT W 10 W 1.00 43.04 OH2 526 -10.129 ATOM 1.459 11 26.434 W WAT W 55.95 OH2 1.00 .527 -12.146 0.323 ATOM 27.878 W 12 WAT W 1.00 52.47 OH2 528 -10.741 MOTA 0.259 31.427 13 W W OH2 WAT 1.00 56.49 529 -6.889 8.411 ATOM 29.889 W OH2 WAT W 1.00 32.19 14 530 -4.021 1.843 ATOM 22.532 W OH2 WAT W 15 1.00 39.56 531 -0.534 -4.336 ATOM 23.814 OH2 WAT W 16 1.00 33.28 W 532 -5.292 1.598 ATOM 19.996 W 17 1.00 28.37 W OH2 WAT 533 -3.040 -8.386 ATOM 25.262 W 18 1.00 30.95 OH2 WAT 534 0.000 0.001 MOTA 22.556 W 19 1.00 29.32 OH2 WAT 535 -1.823 -1.421 ATOM 24.369 W OH2 WAT W 20 1.00 46.18 -6.291 536 ATOM -0.583 29.134 OH2 WAT W 21 1.00 43.67 W 537 -5.533 2.286 ATOM 27.394 W OH2 WAT W 22 1.00 45.47 538 -4.387 MOTA 26.774 0.049 1.00 52.80 OH2 WAT W 23 W 1.507 539 5.236 ATOM 30.008 OH2 WAT W 24 1.00 42.94 W 540 0.356 4.560 MOTA 27.776 OH2 WAT W 25 1.00 53.15 W 0.261 541 6.237 ATOM 32.018 26 W OH2 WAT W 1.00 34.71 542 -0.423 MOTA 4.426 18.650 OH2 WAT W 28 1.00 42.23 W 543 -1.284 ATOM 1.842 18.919 OH2 WAT W 29 W 1.00 59.49 7.700 544 ATOM 6.239 11.826 OH2 WAT W 30 W 1.00 52.76 2.919 545 MOTA 13.683 5.469 W OH2 WAT W 31 1.00 47.84 1.380 546 ATOM 16.956 4.594 32 W OH2 WAT W 1.00 46.32 547 7.679 ATOM 17.260 2.099 OH2 WAT W 33 1.00 51.94 W 548 -4.073 17.636 ATOM 1.737 34 W OH2 WAT W 1.00 30.19 549 9.764 ATOM 5.835 16.221 W OH2 WAT W 35 51.32 8.979 1.00 550 MOTA 8.926 26.030 W 36 OH2 WAT W 1.00 52.05 551 9.624 ATOM 2.898 13.758 37 W OH2 WAT W 1.00 35.86 552 11.925 MOTA 5.914 14.899 W 38 1.00 45.90 OH2 WAT W 553 14.724 MOTA 0.030 19.841 W 39 OH2 WAT W 12.179 1.00 50.60 554 MOTA 13.772 2.335 40 W WAT W 1.00 51.80 OH2 555 6.229 ATOM 0.805 13.367 W WAT W 41 1.00 30.05 OH2 15.845 556 ATOM 3.501 15.587 W TAW 42 W 1.00 48.74 OH2 .557 13.819 ATOM 4.098 14.280 43 W OH2 W TAW 1.00 32.62 558 18.042 ATOM 3.983 14.273 W OH2 WAT W 44 1.00 40.19 559 20.720 ATOM 2.720 14.275 W 45 OH2 WAT W 18.885 1.00 22.32 560 ATOM 2.228 21.969 W 46 1.00 28.43 OH2 WAT W 21.594 561 MOTA 1.778 21.588 47 WAT W 22.023 1.00 50.50 OH2 ATOM 562 3.300 11.908 W 48 OH2 WAT W 18.643 1.00 46.64 563 ATOM 13.679 0.626 49 W TAW 1.00 30.08 OH2 22.597 ATOM 564 2.196 16.369 50 OH2 WAT W 1.00 37.29 18.634 ATOM 565 6.527 12.828 51 OH2 WAT W 1.00 25.55 19.581 ATOM 566 2.631 52 24.603 1.00 58.27 W OH2 WAT W 567 23.131 0.791 ATOM 11.867 1.00 50.24 OH2 WAT W 53 17.812 5.366 568 ATOM 24.646 54 1.00 49.14 OH2 WAT W 17.131 569 0.091 ATOM 20.954 1.00 36.92 OH2 W TAW 55 21.394 570 MOTA 19.747 -0.562 56 WAT W 1.00 33.61 OH2 19.922 571 MOTA 8.442 14.819 57 1.00 45.89 OH2 W TAW 19.724 MOTA 572 5.349 10.854 WAT W 58 1.00 37.52 OH2 573 19.376 MOTA 9.378 10.710 OH2 WAT W 59 1.00 34.96 574 21.845 ATOM 10.303 10.497 60 W WAT OH2 575 MOTA

Figure 7L

Docket/App No.: 0399.1192-008 Inhibitors of HIV Membrane Fusion Title: Debra M. Eckert, et al. ntors:

1.00 28.86 26.354 12.866 5.691 $\mathbb{T} A W$ MOTA 576 OH2 1.00 42.32 25.495 28.773 7.878 10.758 WAT W 62 OH2 MOTA 577 1.00 29.65 1.00 37.31 11.782 6.555 OH2 WAT W 63 578 MOTA 8.472 27.988 10.296 WAT W 579 OH2 W ATOM 1.09 43.22 2.342 26.849 13.316 OHO WAT W 580 ATOM 1.00 38.41 -1.693 28.654 29.863 W TAW THO 66 MOTA 581 W 1.00 32.71 26.444 -1.186 16.468 OH2 WAT W 67 ATOM 582 1.00 18.68 25.212 12.065 OH2 WAT W 20.934 MOTA 583 1.00 48.02 W 26.485 5.989 7.101 OH2 WAT W 69 W ATOM 1.00 33.30 27.574 10.744 7.226 OH2 WAT W 70 585 W ATOM 1.00 34.36 34.997 -1.374 16.382 71 OH2 WAT W ATOM 1.00 28.82 38.167 -0.717 72 17.474 OH2 WAT W 587 W ATOM 1.00 27.39 -2.951 33.186 17.984 OH2 WAT W 73 ATOM 1.00 37.09 37.830 1.929 74 16.999 OHE WAT W 589 W ATOM 39.121 1.00 19.51 3.071 75 20.595 590 OH2 WAT W ATOM 1.00 20.31 39.584 5.004 14.326 76 OH2 WAT W 591 ATOM 38.034 1.00 32.93 11.973 4.544 77 592 OH2 WAT W ATOM 1.00 44.00 39.397 4.417 18.317 78 593 OH2 WAT W MOTA 30.948 1.00 52.39 10.983 -2.804OH2 WAT W 79 594 ATOM 1.00 30.78 0.945 32.640 11.064 OH2 WAT W 80 595 ATOM 39.566 1.00 51.74 0.902 12.861 OH2 WAT W 81 596 ATOM 39.210 1.00 48.06 -1.379 14.353 597 OH2 WAT W 82 MOTA 1.00 46.54 36.263 13.014 -3.417 OH2 WAT W 8.3 598 W ATOM 39.669 1.00 61.24 11.101 -2.319 OH2 WAT W 84 599 ATOM 1.00 26.25 31.838 20.879 -3.825 OH2 WAT W 85 600 W 1.00 36.86 MOTA 28.192 24.470 -4.753 OH2 WAT W 86 601 1.00 38.03 W MOTA 29.831 -5.700 22.117 602 OH2 WAT W 87 1.00 28.21 ATOM W 41.041 0.721 19.685 WAT W 88 OH2 603 ATOM 1.00 32.29 W 40.337 5.127 20.274 WAT W 89 OH2 604 1.00 ATOM 29.943 33.10 W 10.072 4.538 WAT W 90 OH2 605 1.00 33.22 ATOM W 33.496 4.216 10.573 OH2 WAT W 91 ATOM 606 1.00 48.48 W 36.364 10.336 5.922 WAT W 92 OH2 607 1.00 51.71 W ATOM 40.332 9.113 5.209 W TAW 93 608 OH2 1.00 24.98 W ATOM 42.573 9.980 8.713 WAT W 94 OH2 609 1.00 36.93 W ATOM -1.798 6.542 17.708 OH2 W TAW 95 610 W ATOM 1.00 17.13 38.730 11.397 10.278 он2 WAT W 96 1.00 15.62 W ATOM 611 10.478 36.184 11.290 WAT W 97 OH2 ATOM 612 W 1.00 37.395 12.988 8.444 WAT W 98 OH2 1.00 25.18 W ATOM 613 40.361 8.735 9.911 WAT W 99 OHE ATOM 614 1.00 28.95 W 35.865 11.917 6.665 OH2 WAT W 100 ATOM 615 1.00 28.77 w 8.907 9.736 35.113 WAT W 101 OH2 ATOM 616 W 1.00 32.80 42.300 10.416 5.919 OH2 WAT W 102 ATOM 617 W 1.00 54.85 3.600 38.536 8.278 OH2 WAT W 103 ATOM 618 W 1.00 23.53 7.249 45.734 14.183 OH2 WAT W 104 ATOM 619 1.00 34.68 46.547 7.965 11.426 OH2 WAT W 105 MOTA 620 W 1.00 39.50 2.218 41.970 16.907 OH2 WAT W 106 ATOM 621 1.00 23.72 W 46.761 16.479 14.336 OH2 WAT W 107 MOTA 622 1.00 22.11 W 12.931 45.022 8.319 OH2 WAT W 108 ATOM 623 1.00 39.34 W 12.423 42.385 7.189 OH2 WAT W 109 624 W ATOM 1.00 40.15 9.769 44.603 8.599 OH2 WAT W 110 625 ATOM 1.00 23.69 -1.858 33.829 26.891 OH2 WAT W 111 626 ATOM 1.00 38.13 32.521 -3.310 28.775 OH2 WAT W 112 627 ATOM 1.00 34.37 33.068 0.587 31.335 OH2 WAT W 113 628 ATOM 1.00 44.24 36.513 -0.919 OH2 WAT W 114 30.921 629 1.00 39.50 ATOM 29.619 2.733 30.098 OH2 WAT W 115 ATOM 530 1.00 52.27 W 34.521 2.665 OH2 WAT W 116 33.465 631 ATOM 1.00 56.10 14.159 -18.301 25.612 OH2 WAT W 117 632 MOTA 1.00 57.70 2.165 -15.960

Figure 7M

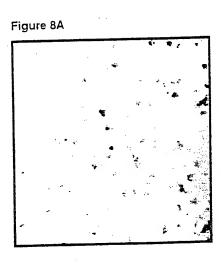
33.904

OH2 WAT W 118

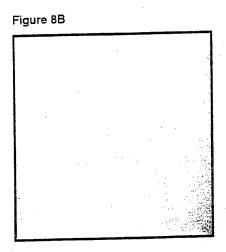
ATOM

ATOM	634	онг	WAT	W	119	33.766		-14.106		57.44 40.38	W W
ATOM	635	OH2	WAT	W.	120	26.831	7.497	7.075		32.00	W
ATOM	636	OH2	WAT	W	121	26.562	8.206	4.240		46.30	W
ATOM	637	OH2	TAW	W	122	29.081	7.039	3.251			W
ATOM	638	OH2	WAT	W	123	22.080	-0.975	10.516		39.31	W
ATOM	639	OH2	WAT	W	124	28.185	3.991	13.044		45.28 52.21	W
ATOM	640	OH2	WAT	W	125	29.400	7.324	10.996			W
ATOM	641	OH2	WAT	W	126	12.966	3.595	24.673		59.42 45.85	W
ATOM	642	OH2	TAW	W	127	8.932	7.961	36.476			W
ATOM	643	OH2		W	128	12.712	5.206	41.719		38.55	W
ATOM	644	OH2	WAT	W	129	9.431	10.564	47.230		35.27	W
ATOM	645	OH2	WAT		130	6.643	9.576	45.596		44.00	W
ATOM	646	OH2	WAT		131	21.501	13.657	45.856		43.49 41.15	W
ATOM	647	OH2			132	19.368	14.112	46.567		36.86	W
ATOM	648	OH2		W	133	20.913	12.058	48.230		49.55	W
ATOM	649	OH2	WAT	W	134	13.556	4.967	44.137	1.00	54.94	W
ATOM	650	OH2	WAT	W	135	17.568	0.000	0.010		42.03	W
ATOM	651	OH2	WAT	W	136	17.847	-0.139	11.093		35.36	W
ATOM	652	OH2	WAT	W	137	25.734	4.074	15.641		37.47	W
ATOM	653	OH2	WAT	W	138	8.107	7.930	38.831 44.378		61.10	W
ATOM	654	OH2	WAT	W	139	10.614	4.603	32.610		37.66	W
ATOM	655	OH2	WAT	W	140	14.180	-9.552	22.858		48.05	W
ATOM	656	OH2	WAT	W	141	26.549	-4.072	22.856		36.75	W
ATOM	657	OH2	WAT	W	142	21.688	-2.141	27.799		38.11	W
ATOM	658	OH2	TAW	W	143	15.457	1.462	45.521		36.93	W
ATOM	659	OH2	TAW	W	144	18.956	16.356	40.183		40.77	W
ATOM	660	OH2	WAT	W	145	15.655	2.938	19.777		47.04	W
ATOM	661	OH2	WAT	W	146	15.688	-1.613	28.327		44.89	W
ATOM	662	OH2		W		26.880	-5.627	33.707		43.34	W
MOTA	663	OH2	TAW	W		28.682	-5.605			53.67	W
ATOM	664	OH	TAW			28.220	11.179	-7.774		44.54	W
MOTA	665	OH2	TAW S	W	150	27.905	3.222			47.59	W
MOTA	666	OH2	TAW S	W	151	15.403	-11.541	34.333	1.00	4,.55	
TER											
END											

Inhibition of HIV-1 Membrane Fusion by a D-Peptide



Syncytia Assay with no D-peptide



Syncytia Assay with [100 μM] peptide

Docket/App No.. 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion

Debra M. Eckert, et al. Inventors:

NMR Charact rization of Aromatic Residues in **IQN17/D-Peptide Complexes**

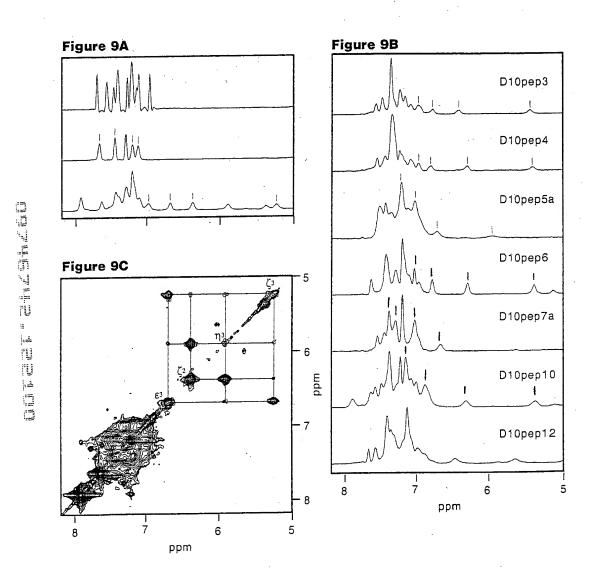
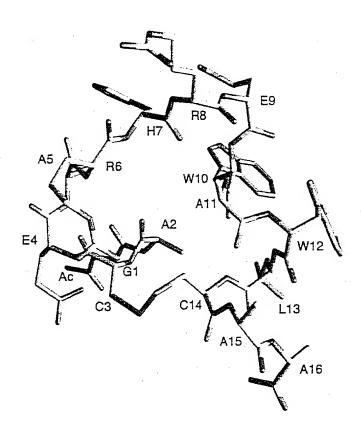


Figure 10: Conformation of D10pep1 in complex with IQN17



Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion

Inventors: Debra M. Eckert, et al.

CRYST1	57	. 935	121	9 !	59 73.6	69	90.	00	90.00	90.00	C2221		1	
ORIGX1		1.00	0000) (0.000000	0.	.0000	00		0.00000)			
ORIGX2		0.00	0000	:	1.000000	0.	0000	00		0.00000)			
ORIGX3		0.00	0000	(0.000000	1.	0000	00		0.0000)			
SCALE1		0.01	7261	. (0.000000	0.	0000	0.0		0.00000				
SCALE2			0000		0.008199		00000			0.00000				
SCALE3			0000		0.000000		0135			0.00000				
ATOM	1	CA	ACE		0		.795		.140	37.286		61.88		. 3
ATOM	2	C	ACE		0		799		.376	36.435		62.00		A
ATOM	3	0			0		5.500							A
	4	-	ACE		-				.475	36.921		62.10		A
ATOM	_		ARG		1		.134		.217	35.157		60.34		A
ATOM	5.	CA	ARG		1		.203		.328	34.217		60.56		A
ATOM	6	CB	ARG		1		.212		.993	33.110		61.87		A
ATOM	7	CG	ARG		1		.630		.135	32.212		60.78		A
ATOM	8	CD	ARG		1		.500		.587	31.097		64.25		A
ATOM	9	NE	ARG		1		.018		.628	30.217		65.07		A
ATOM	10	CZ	ARG	A	1	29	.706	20	. 377	29.109	1.00	63.90		A
ATOM	11		ARG		1	29	.951	19	.124	28:766	1.00	64.20		A
ATOM	12	NH2	ARG	Α	1	30	.157	21	.367	28.351	1.00	63.51		A
ATOM	13	C	ARG	Α	1	24	.823	19	.573	33.595	1.00	59.45		A
ATOM	14	0	ARG	A	1	24	.453	20	.714	33.294	1.00	57.69		A
ATOM	15	N	MET	Α	2 .	24	.065	18	.494	33.425	1.00	57.60		A
ATOM	16	CA	MET	Α	2	22	.736	18	.573	32.836	1.00	59.35		A
ATOM	17	CB	MET	Α	2	22	.273	17	.198	32.397		59.85		. A
ATOM	18	CG	MET	A	2		.204		.251	31.342		63.56		A
ATOM	19	SD	MET	A	2		.044		.905	31.454		67.77		A
ATOM	20	CE	MET	A	2		.089		.438	32.857		66.61		A
ATOM	21	c	MET	A	2		.723		.130	33.834		61.33		A
ATOM	22	ō	MET	A	2		.543		.276	33.521		59.97		A
ATOM	23	N	LYS	A	3		.200		.417	35.041		62.71		A
ATOM	24	CA	LYS		3		.373		.961	36.107		63.07		
ATOM	25	CB	LYS	Ā	3		.817							A
ATOM	26	CG		A	3				.361	37.449		64.25		A
							.982		.721	38.687		64.89		A
ATOM	27 28	CD	LYS				.195		.159	39.160		64.67		A
ATOM		CE	LYS	A	3		.543		.405	40.525		64.66		A
ATOM	29	NZ	LYS		3 .		.077		. 123	40.548		63.04		A
ATOM	30	C	LYS	A	3		.599		. 467	36.062		64.55		A
ATOM	31	0	LYS		3		.639		. 245	36.032		64.65		А
ATOM	32	N	GLN		4		.869		. 873	36.036		64.34		A
ATOM	33	CA	GLN	A	4		.232		.289	35.952		65:46		A
ATOM	34	CB	GLN		4		.746		. 447	35.780		67.71		A.
MOTA	35	CG	GLN		4		.552		.954	36.963		71.16		A
ATOM	36	CD	GLN		4		.297		.771	38.212		75.18		A
ATOM	3.7		GLN		4		.618		.962	38.269	1.00			A
MOTA	38		GLN		4		.706		.135	39.225	1.00			A
MOTA	39	С	GLN	A	4	22	.508	23.	928	34.758	1.00	64.11		A
ATOM	40	0	GLN	А	4	22.	.191	25.	128	34.776	1.00	62.08		A
ATOM	41	N	ILE	A	5	22.	.260	23.	120	33.726	1.00	59.80		A
ATOM	42	CA	ILE	A	5	21.	.540	23.	587	32.552	1.00	58.22		A
ATOM	43	CB	ILE	A	5 ·	21.	.567	22.	558	31.398	1.00	56.85		A
ATOM	44	CG2	ILE	Α	5	20.	438	22.	851	30.416	1.00	53.92		A
ATOM	45	CG1	ILE	A	5	22.	942	22.	562	30.719	1.00	56.47		A
ATOM	46	CD1		A	5		079		524	29.514	1.00			A
ATOM	47	C	ILE	A	5		083		328	32.929	1.00			A
ATOM	48	5		A	5		575		928	32.729	1.00			A
ATCM	49	И		A	6		424		796	33.472	1.00			A
ATOM	50	CA	GLU		ő		013		383	33.377	1.00			A
ATCM	51	CB	GLU		6		528		537	34.448	1.00			A
-14 017	-		320		5	± , .			, ,	J4.140	00			Α.

Figure 11A

ATOM	52 CG GLUA 6	17.638 20.359 33.480 1.00 56.46	
ATOM	53 CD GLUA 6	15 20 20 40	A
ATOM	54 OE1 GLU A 6	17 700 10 700 00 00	A
ATOM	55 OE2 GLU A 6	16 544 10 155	A
ATOM	56 C GLU A 6	15 000 000 000	A
ATOM	57 O GLU A 6	16 700 84 700	A
ATOM	58 N ASP A 7	70 706	A
ATOM	59 CA ASP A 7	10 000 00 000 00	A
ATOM	60 CB ASP A 7	20 201	· A
ATOM	61 CG ASP A 7	2.00 37.40	A
ATOM	62 OD1 ASP A 7	2.00 37.37	A
ATOM	63 OD2 ASP A 7	19.180 23.534 38.775 1.00 53.78	. A
ATOM	64 C ASPA 7	20.637 24.862 39.771 1.00 57.66	A
ATOM	65 O ASP A 7	19.034 26.745 36.041 1.00 56.99	· A
ATOM	66 N LYS A 8	18.516 27.662 36.678 1.00 55.43	A
ATOM	67 CA LYS A 8	19.632 26.945 34.873 1.00 58.30	A
ATOM		19.642 28.290 34.312 1.00 59.87	A
ATOM		20.971 28.599 33.612 1.00 62.61	A
MOTA	•	22.203 28.372.34.487 1.00 66.85	A
ATOM		23.232 29.498 34.357 1.00 70.21	A
ATOM	•	22.915 30.676 35.293 1.00 72.00	A
ATOM		21.583 31.323 35.091 1.00 72.05	A
	73 C LYS A 8	18.467 28.481 33.354 1.00 58.08	A
ATOM	74 O LYS A 8	18.145 29.609 32.969 1.00 56.44	A
ATOM	75 N ILE A 9	17.835 27.376 32.967 1.00 55.29	A
ATOM	76 CA ILE A 9	16.668 27.436 32.099 1.00 56.69	A
ATOM	77 CB ILE A 9	16.325 26.052 31.486 1.00 54.89	Α
ATOM	78 CG2 ILE A 9	14.892 26.067 30.915 1.00 54.20	A
ATOM	79 CG1 ILE A 9	17.373 25.676 30.423 1.00 55.96	A
ATOM	80 CD1 ILE A 9	17.131 24.339 29.717 1.00 54.22	A
ATOM	81 C ILE A 9	15.526 27.876 33.018 1.00 57.98	A
ATOM	82 O ILE A 9	14.603 28.572 32.616 1.00 55.85	A
ATOM	83 N GLUA 10	15.626 27.458 34.271 1.00 59.96	A
MOTA	84 CA GLU A 10	14.641 27.788 35.283 1.00 61.12	· A
ATOM	85 CB GLU A 10	14.850 26.901 36.510 1.00 63.01	A
ATOM	86 CG GLU A 10	13.846 27.117 37.618 1.00 66.89	A
ATOM	87 CD GLU A 10	14.387 26.672 38.955 1.00 68.37	A
ATOM	88 OE1 GLU A 10 ·	14.844 25.510 39.054 1.00 67.70	. A
ATOM	89 OE2 GLU A 10	14.355 27.487 39.903 1.00 68.42	A
ATOM	90 C GLUA 10	14.872 29.243 35.664 1.00 59.41	A
ATOM	91 O GLUA 10	13.947 29.958 36.037 1.00 59.95	A
ATOM	92 N GLUA 11	16.127 29.663 35.565 1.00 57.16	A
ATOM	93 CA GLU A 11	16.524 31.024 35.893 1.00 55.88	A
ATOM	94 CB GLU A 11	18.042 31.095 36.019 1.00 58.17	A
ATOM	95 CG GLU A 11	18.569 32.375 36.627 1.00 62.73	A
ATOM	96 CD GLU A 11	18.459 32.382 38.139 1.00 67.75	A
ATOM	97 OE1 GLU A 11	19.101 31.512 38.782 1.00 67.91	A
MOTA	98 OE2 GLU A 11	17.736 33.249 38.681 1.00 68.84	A
ATOM	99 C GLUA 11	16.056 31.976 34.789 1.00 54.76	A
ATOM	100 O GLU A 11	15.805 33.160 35.030 1.00 54.78	A
ATOM	101 N ILE A 12	15.945 31.443 33.575 1.00 52.61	A
ATOM	102 CA ILE A 12	15.510 32.210 32.414 1.00 50.09	A
ATOM	103 CB ILE A 12	16.002 31.548 31.096 1.00 50.23	A
ATOM	104 CG2 ILE A 12	15.201 32.073 29.905 1.00 48.54	A
ATOM	105 CG1 ILE A 12	17.508 31.773 30.930 1.00 50.30	A
MOTA	106 CD1 ILE A 12	18.114 31.062 29.724 1.00 53.10	A
MOTA	107 C ILE A 12	13.988 32.324 32.362 1.00 49.83	A
ATOM	108 O ILE A 12	13.447 33.376 32.017 1.00 47.70	A
MCTA	109 N GLUA 13	13.306 31.232 32.698 1.00 48.57	A
ATOM	110 CA GLU A 13	11.849 31.218 32.577 1.00 48.22	A
MOTA	111 CB GLU A 13	11.320 29.810 32.954 1.00 45.44	A
			Ω.

Figure 11B

ATOM	112 CG GLU A 13	11.673 28.794 31.895 1.00 46.65	
ATOM	113 CD GLU A 13	11.419 27.372 32.358 1.00 49.90	Α
ATOM	114 OE1 GLU A 13	12.051 26.968 33.366 1.00 49.96	A
ATOM	115 OE2 GLU A 13	10.599 26.665 31.720 1.00 50.18	A
ATOM	116 C GLU A 13	11.357 32.163 33.749 1.00 47.83	A
ATOM	117 O GLU A 13	10.279 32.731 33.638 1.00 48.72	A
ATOM	118 N SER A 14	12.168 32.313 34.786 1.00 48.67	A
ATOM	119 CA SER A 14	11.862 33.187 35.907 1.00 49.89	A A
ATOM	120 CB SER A 14	12.906 32.985 37.014 1.00 49.05	. A
MOTA	121 OG SER A 14	12.634 33.773 38.160 1.00 49.35	A
ATOM	122 C SER A 14	11.885 34.627 35.415 1.00 50.52	A
ATOM	123 O SER A 14	10.869 35.313 35.431 1.00 54.15	A
ATOM	124 N LYS A 15	13.056 35.067 34.971 1.00 49.27	A
ATOM	125 CA LYS A 15	13.248 36.416 34.474 1.00 51.02	A
ATOM	126 CB LYS A 15	14.707 36.589 34.042 1.00 54.30	A
ATOM ATOM	127 CG LYS A 15	15.018 37.931 33.417 1.00 58.79	A
	128 CD LYS A 15	14.843 39.039 34.437 1.00 63.42	A
ATOM ATOM	129 CE LYS A 15	15.841 38.880 35.576 1.00 65.66	A
ATOM	130 NZ LYS A 15	15.722 39.983 36.569 1.00 68.14	A
ATOM	131 C LYS A 15	12.313 36.758 33.305 1.00 50.99	A
ATOM	132 O LYS A 15 133 N GLN A 16	12.022 37.926 33.061 1.00 49.62	A
ATOM		11.848 35.740 32.587 1.00 50.06	A
ATOM		10.965 35.937 31.444 1.00 49.96	A
ATOM		10.950 34.684 30.570 1.00 49.89	A
ATOM		10.133 34.810 29.286 1.00 50.59	A
ATOM	137 CD GLN A 16 138 OE1 GLN A 16	10.287 33.603 28.369 1.00 54.27	A
ATOM		9.799 32.511 28.667 1.00 56.28	A
ATOM	139 NE2 GLN A 16 140 C GLN A 16	10.985 33.796 27.250 1.00 54.69	A
ATOM	141 O GLN A 16	9.551 36.256 31.899 1.00 50.61	Α
ATOM	142 N LYS A 17	8.788 36.931 31.195 1.00 48.56 9.198 35.736 33.067 1.00 48.38	A
ATOM	143 CA LYS A 17	7 000	A
ATOM	144 CB LYS A 17	2.00 45.75	A
ATOM	145 CG LYS A 17	5 750 75 757	A
ATOM	146 CD LYS A 17	1.00 36.86	A
ATOM	147 CE LYS A 17	1.00 33.31	A
ATOM	148 NZ LYS A 17	. 500	A
ATOM	149 C LYS A 17	2.00 02.03	A
ATOM	150 O LYS A 17	7.927 37.390 34.163 1.00 48.25 6.977 38.144 34.008 1.00 47.73	A
ATOM	151 N LYS A 18	9.043 37.750 34.791 1.00 45.58	A
MOTA	152 CA LYS A 18	9.190 39.101 35.309 1.00 45.26	A
MOTA	153 CB LYS A 18	10.523 39.270 36.047 1.00 47.34	A
ATOM	154 CG LYS A 18	10.627 38.493 37.362 1.00 50.10	A
ATOM	155 CD LYS A 18	11.831 38.976 38.168 1.00 52.93	'A A
ATOM	156 CE LYS A 18	11.869 38.358 39.550 1.00 55.07	Ā
MOTA	157 NZ LYS A 18	12.933 38.968 40.398 1.00 59.20	A
ATOM	158 C LYS A 18	9.107 40.110 34.171 1.00 41.59	A
ATOM	159 O LYS A 18	8.585 41.206 34.349 1.00 42.70	- A
ATOM	160 N ILE A 19	9.633 39.740 33.008 1.00 40.25	A
ATOM	161 CA ILE A 19	9.605 40.595 31.831 1.00 39.53	A
ATOM ATOM	162 CB ILE A 19	10.494 40.015 30.710 1.00 42.08	A
	163 CG2 ILE A 19	10.133 40.631 29.369 1.00 41.71	A
ATOM ATÓM	164 CG1 ILE A 19	11.969 40.214 31.074 1.00 42.52	A
ATOM	165 CD1 ILE A 19 166 C ILE A 19	12.939 39.656 30.039 1.00 43.29	A
ATOM		8.172 40.725 31.325 1.00 39.27	A
ATOM		7.751 41.790 30.899 1.00 37.81	. A
ATOM		7.421 39.637 31.372 1.00 39.00	A
ATOM		6.036 39.692 30.930 1.00 40.27	A
ATOM		5.437 38.280 30.834 1.00 43.21	A
011	171 CG GLU A 20	5.898 37.474 29.606 1.00 48.10	A

Figure 11C

MOTA	172	CD	GLU	A	20	5.446	36.019	29.659	1.00 50.57	A
MOTA	173		GLU		20	5.832	35.316	30.617	1.00 52.42	A
ATOM	174		GLU		20	4.708	35.575	28:752	1.00 52.16	A
ATOM	175	С	GLU		20	5.195	40.546	31.873	1.00 40.09	A
ATOM	176	ō	GLÜ		20	4.148	41.056	31.480	1.00 40.96	A
ATOM	177	N	ASN		21	5.637	40.694	33.119	1.00 38.83	A
ATOM	178	CA	ASN		21	4.880	41.498	34.071	1.00 40.69	A
	179	СВ	ASN		21	5.216	41.107	35.507	1.00 39.42	A
ATOM ATOM	180	CG	ASN		21	4.618	39.768	35.892	1.00 41.35	A
ATOM	181	OD1			21	3.905	39.151	35.102	1.00 38.98	. A
ATOM	182		ASN		21	4.902	39.312	37.107	1.00 40.82	A
ATOM	183	C	ASN		21	5.163	42.958	33.846	1.00 42.25	A
ATOM	184	0	ASN		21	4.261	43.801	33.872	1.00 42.61	A
MOTA	185	N	GLU		22	6.432	43.244	33.602	1.00 41.94	A
MOTA	186	CA	GLU		22	6.893	44.589	33.343	1.00 41.44	A
ATOM	187	CB	GLU		22	8.403	44.563	33.127	1.00 43.01	A
ATOM	188	CG	GLU		22	9.126	45.861	33.421	1.00 49.75	A
ATOM	189	CD	GLU		22	9.769	45.872	34.802	1.00 52.80	· A
ATOM	190		GLU		22	10.611	44.988	35.077	1.00 53.66	A
ATOM	191		GLU		22	9.447	46.764	35.608	1.00 57.41	A
ATOM .	192	C	GLU		22	6.188	45.082	32.068	1.00 41.34	A
ATOM	193	ō	GLU		22	5.851	46.263	31.954	1.00 43.52	A
ATOM	194	N		A	23	5.964	44.175	31.116	1.00 37.55	A
ATOM	195	CA	ILE	A	23	5.295	44.530	29.863	1.00 35.10	A
ATOM	196	CB	ILE		23 -	5.418	43.408	28.800	1.00 36.19	A
ATOM	197	CG2	ILE		23	4.520	43.719	27.592	1.00 35.94	A
ATOM	198	CG1			23	6.876	43.288	28.340	1.00 39.18	A
ATOM	199		ILE		23	7.122	42.193	27.324	1.00 40.80	A
ATOM	200	С	ILE		23	3.816	44.827	30.093	1.00 33.36	A
ATOM	201	ō	ILE		23	3.284	45.796	29.568	1.00 28.55	A
MOTA	202	N	ALA		24	3.167	43.981	30.881	1.00 30.41	A
ATOM	203	ÇA	ALA		24	1.760	44.147	31.179	1.00 30.11	A
ATOM	2.04	CB	ALA		24	1.276	42.994	32.043	1.00 27.29	A
ATOM	205	C	ALA	A	24	1.531	45.479	31.893	1.00 31.41	A
ATOM	206	0	ALA	A	24	0.562	46.183	31.608	1.00 31.49	A
ATOM	207	N	ARG	Α	25	2.428	45.825	32.816	1.00 30.94	A
ATOM	208	CA	ARG	A	25	2.297	47.070	33.547	1.00 30.44	A
ATOM	209	CB	ARG	Α	25	3.197	47.066	34.798	1.00 32.01	A
ATOM	210	CG	ARG	A	25	2.727	46.101	35.894	1.00 34.49	A
ATOM	211	CD -	ARG	A	25	3.471	46.326	37.218	1.00 39.65	A A
ATOM	212	NE	ARG	A	25	4.873	45.907	37.177	1.00 40.74	A A
ATOM	213	CZ	ARG	A	25	5.308	.44.687	37.496	1.00 43.06	A
MOTA	214	NHl	ARG	А	25	4.453	43.749	37.885	1.00 39.85	A
ATOM	215	NH2	ARG	A	25	6.606	44.399	37.399	1.00 40.30 1.00 28.86	A
ATOM	216	. C	ARG	Α	25	2.590	48.270	32,651		A
ATOM	217	0	ARG		25	1.907	49.296	32.728	1.00 29.35 1.00 26.96	A
MOTA	218	N	ILE		26	3.587	48.147	31.790	1.00 28.98	Ā
ATOM	219	CA	ILE		26	3.917	49.226	30.875	1.00 28.43	A
ATOM	220	CB	ILE		26	5.132	48.832	29.990	1.00 25.38	A
ATOM	221	CG2			26	5.239	49.760	28.799	1.00 28.70	A
ATOM	222	CG1			26	6.414	48.835	30.839	1.00 27.77	A
ATOM	223	CD1			26	7.546	48.257	30.132	1.00 27.77	Ā
ATOM	224	C	ILE		26	2.719	49.571	29.968	1.00 30.92	A
ATOM	225	0	ILE		26	2.425	50.746	29.690	1.00 32.33	Ā
ATOM	226	N	LYS		27	2.019	48.540	29.512	1.00 30.30	Ä
ATOM	227	CA	LYS		27	0.887	48.730	28.627	1.00 33.83	Ā
ATOM	228	CB	LYS		27	0.449	47.388	28.045 27.185	1.00 33.83	A
ATOM	229	CG	LYS		27	1.520	46.729		1.00 39.84	. A
ATOM	230	CD	LYS		27	1.167	45.294	26.831	1.00 44.41	A
ATOM	231	CE	LYS	À	27	-0.086	45.204	26.003	1.00 40.04	

Figure 11D

Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion Inventors: Debra M. Eckert, et al.

ATOM	232	NZ	LYS	A	27 -	-0.384	43.774	25.698	1.00 53.94	A
ATOM	233	С	LYS	Α	27	-0.267	49.402	29.344	1.00 28.67	A
MOTA	234	0	LYS	A	27	-0.919	50.252	28.767	1.00 26.05	A A
ATOM	235	N	LYS		28	-0.511	49.020	30.593	1.00 27.68	A
MOTA	236	CA		A	28	-1.597	49.609	31.371	1.00 27.30 1.00 24.82	A
ATOM	237	CB	LYS		28	-1.797	48.845	32.691 33.573	1.00 24.82	A
ATOM	238	ÇG		Α	28	-2.961	49.384	32,744	1.00 31.59	A
ATOM	239	CD		A	28	-4.263	49.506	33.606	1.00 30.02	A
MOTA	240	CE	LYS		28	-5.526	49.699 50.820	34.586	1.00 31.11	A
ATOM	241	NZ	LYS		28	-5.440 -1.284	51.076	31.641	1.00 29.57	·A
ATOM	242	C	LYS		28 28	-2.164	51.951	31.566	1.00 28.21	A
ATOM	243	0	LYS LEU		29	-0.017	51.359	31.923	1.00 29.36	A
ATOM	244	N CA	LEU		29	0.385	52.723	32.179	1.00 33.70	A
MOTA	245 246	CB	LEU		29	1.822	52.745	32.692	1.00 35.26	A
ATOM	247	CG	LEU		29	2.023	53.727	33.847	1.00 38.04	A
MOTA MOTA	248		LEU		29	3.363	53.485	34.506	1.00 39.85	A
ATOM	249		LEU		29	1.891	55.149	33.332	1.00 38.01	A
ATOM	250	C	LEU		29	0.243	53.561	30.905	1.00 34.59	A
ATOM	251	ō	LEU		29	-0.281	54.691	30.927	1.00 37.16	A
ATOM	252	N	LEU		30	0.721	53.020	29.792	1.00 34.03	A
ATOM	253	CA	LEU	A	30	0.616	53.724	28.528	1.00 35.56	A
ATOM	254	CB	LEU	A	30	1.230	52.874	27.414	1.00 38.09	A
ATOM	255	CG	LEU	Α	30	1.470	53.508	26.050	1.00 40.19	A A
MOTA	256	CD1	LEU	Α	30.	2.270	54.805	26.163	1.00 39.79 1.00 45.44	A
ATOM	257		LEU		30	2.215	52.484	25.198 28.263	1.00 45.44 1.00 34.76	A
MOTA	258	C	LEU		30	-0.882	53.980	27.794	1.00 34.70	A
ATOM	259	0	LEU		30	-1.269	55.050 52.996	28.572	1.00 30.55	A
MOTA	260	N	GLN		31	-1.713 -3.152	53.142	28.401	1.00 31.04	A
MOTA	261	CA	GLN		31	-3.152	51.839	28.782	1.00 33.01	A
ATOM	262	CB	GLN		31 31	-5.397	51.924	28.839	1.00 37.09	A
ATOM	263	CG CD	GLN GLN		31	-6.045	50.582	29.159	1.00 45.53	A
ATOM	264	OE1			31	-5.715	49.940	30.159	1.00 52.72	Α
ATOM ATOM	265 266	NE2			31	-6.973	50.151	28.310	1.00 46.91	A
ATOM	267	C	GLN		31	-3.633	54.303	29.273	1.00 31.34	A
ATOM	268	ō	GLN		31	-4.419	55.125	28.832	1.00 28.45	, A
ATOM	269	N	LEU		32	-3.141	54.376	30.509	1.00 30.93	A
ATOM	270	CA	LEU	A	- 32	-3.523	55.459	31.393	1.00 30.83	A
ATOM	271	CB	LEU	A	32	-2.988	*55.237	32.811	1.00 29.49	A A
ATOM	272	CG	LEU	Α	32	-3.572	54.156	33.732	1.00 31.79 1.00 33.29	A
ATOM	273		LEU		32	-2.810	54.215	35:075	1.00 33.29	A
ATOM	274		LEU		32	-5.058	54.376	33.972 30.860	1.00 32.26	A
ATOM	275	C	LEU		32	-3.031	56.797 57.810	31.031	1.00 35.77	A
ATOM	276	0	LEU		32	-3.707 -1.872	56.798	30.198	1.00 31.70	A
ATOM	277	N	THR		33	-1.298	58.019	29.640	1.00 33.33	A
MOTA	278	CA.	THR		33	0.158	57.787	29.156	1.00 35.07	A
ATOM	279	CB	THR THR		33 33	0.949	57.272	30.238	1.00 39.00	A
ATOM	280	OG1			33	0.776	59.087	28.687	1.00 34.58	A
ATOM	281 282	C	THR		33	-2.120	58.560	28.471	1.00 33.63	A
ATOM	283	0	THE		33	-2.237	59.767	28.298	1.00 33.87	A
ATOM ATOM	284	N	VAL		34	-2.682	57.660	27.670	1.00 35.32	A
ATOM	285	CA	VAL		34	-3.507	58.046	26.531	1.00 36.90	A
ATOM	286	CB	VAL		34	-3.810	56.832	25.622	1.00 36.47	A
ATOM	287	CG1			34	-4.825	57.200	24.550	1.00 34.36	A
ATOM	288	CG:			34	-2.514	56.354	24.966	1.00 38.97	A
ATOM	289	С	VAL		34	-4.809	58.655	27.036	1.00 37.01	· A
ATOM	290	0	VAL		34	-5.250	59.695	26.540	1.00 35.59	A
ATOM	291	N	, TRF	A	35	-5.403	57.992	28.022	1.00 36.34	A

Figure 11E

ATOM	292	CA	מַקַיַּ	A	35	-6.645	58.429	28.648	1.00 38.95	A
ATOM	293	CB	TRP		35	-7.022	57.429	29.742	1.00 44.03	A
ATOM	294	CG	TRP	A	35	-8.302	57.716	30.478	1.00 45.10	A
MOTA	295	CD2		A	3.5	-8.445	58.535	31.640	1.00 46.19	· A
ATOM	296	CE2		A	35	-9.820	58.545	31.973	1.00 47.39	A
ATOM	297	CE3		A	35	-7.556	59.277	32.429		
ATOM	298	CD1		A	35	-9.549	57.260	30.166		Α.
									1.00 45.42	A
MOTA	299.	NE1		A	35	-10.468	57.752	31.063	1.00 47.75	A
MOTA	300	CZ2			35	-10.317	59.258	33.067	1.00 48.12	A
ATOM	301	CZ3			35	-8.049	59.991	33.509	1.00 44.34	A
MOTA	302	CH2		A.	35	-9.419	59.968	33.824	1.00 47.03	Α.
ATOM	303	C	TRP	A	35	-6.408	59.814	29.259	1.00 40.04	A
ATOM	304	0	TRP	Α	35	-7.155	60.759	29.013	1.00 39.15	A
ATOM	305	N	GLY	A	36	-5.352	59.934	30.055	1.00 38.98	A
ATOM	306	CA	GLY	Α	36	-5.039	61.211	30.658	1.00 38.44	A
ATOM	307 .	С	GLY		36	-5.034	62.327	29.634	1.00 38.41	A
ATOM	308	ō	GLY		36	-5.626	63.390	29.845	1.00 40.58	A
ATOM	309	N	ILE	A	37	-4.356	62.094	28.517	1.00 39.01	A
ATOM	310	CA	ILE		37	-4.279	63.079	27.451		
				Α					1,00 40.60	A
ATOM	311	CB	ILE	A	37	-3.395	62.584	26.301	1.00 40.20	A
ATOM	312	CG2		A	37	-3.509	63.517	25.136	1.00 39.97	A
ATOM	313	CGl		A	37	-1.939	62.477	26.767	1.00 41.25	A
ATOM	314	CD1			37	-1.036	61.777	25.778	1.00 38.31	A
MOTA	315	C	ILE	A	37	-5.662	63.366	26.886	1.00 42.00	A
ATOM	316	0	ILE	Α	37	-6.019	64.516	26.654	1.00 42.52	A
ATOM	317	N	LYS	Α	38	-6.438	62.317	26.660	1.00 42.56	A
ATOM	318	CA	LYS	Α	38	-7.766	62.505	26.112	1.00 45.16	A
ATOM	319	CB	LYS	Α	38	-8.459	61.156	25.925	1.00 46.50	A
ATOM	320	CG		A	38	-9.683	61.235	25.026	1.00 53.52	A
ATOM	321	CD		A	38	-10.840	62.017	25,651	1.00 55.55	A
ATOM	322	CE		A	38	-11.812	62.480	24.581	1.00 56.01	A
ATOM	323	NZ	LYS		38	-11.165	63.504	23.714	1.00 55.27	. A
ATOM	324	C		A	38	-8.594	63.405	27.025		
ATOM	325				38	-9.237	64.343		1.00 46.34	A
		0		A				26.561	1.00 48.52	A
ATOM	326	N	GLN		39	-8.554	63.120	28.322	1.00 47.82	A
ATOM	327	CA	GLN		39	-9.303	63.877	29.318	1.00 49.21	A
ATOM	328	CB	GLN		39	-9.142	63.230	30.691	1.00 52.07	A
ATOM	329	CG	GLN		39 .	-9.431	61.742	30.727	1.00 59.01	A
ATOM	330	CD	GLN		39	-10.889	61.409	30.513	1.00 61.01	A
MOTA	331	OE1			39	-11.742	61.800	31.310	1.00 63.56	A
MOTA	332	NE2	GLN	Α	39	-11.188	60.677	29.437	1.00 62.00	A
MOTA	333	C	GLN	A	39	-8.840	65.324	29.412	1.00 48.78	A
MOTA	334	0	GLN	Α	39	-9.649	66.243	29.431	1.00 48.03	A
ATOM	335	N	LEU	A	40	-7.530	65.522	29.472	1.00 49.67	A
ATOM	336	CA	LEU	A	40	-6.980	66.861	29.590	1.00 50.78	A
ATOM	337	CB	LEU	A	40	-5.479	66.785	29.868	1.00 49.62	A
ATOM	338	CG	LEU	A	40	-4.736	68.118	29.982	1.00 47.99	A
ATOM	339	CD1	LEU	A	40	-5.416	69.030	31.011	1.00 51.32	A
ATOM	340		LEU		40	-3.300	67.852	30.376	1.00 48.82	A
ATOM	341	c	LEU		40	-7.227	67.736	28.363	1.00 53.20	A
ATOM	342	0	LEU		40	-7.230	68.964	28.457	1.00 53.20	A
ATOM	343	N	GLN		41	-7.433	67.104	27.215	1.00 56.61	
	344							25.994		A
ATOM		CA	GLN		41	-7.649	67.850		1.00 60.81	A
ATOM	345	CB	GLN		41	-7.295	66.994	24.781	1.00 60.00	A
ATOM	346	CG	GLN		41	-7.257	67.753	23.467	1.00 61.60	A
ATOM	347	CD	GLN		41	-6.756	66.885	22.330.	1.00 61.14	A
ATOM	348	OE1	GLN		41	-5.630	66.377	22.367	1.00 56.12	A
ATOM	349	NE2	GLN	A	41	-7.598	66.697	21.316	1.00 60.61	A
ATOM	350	С	GLN	A	41	-9.084	68.344	25.915	1.00 63.54	A
ATOM	351	0	GLN	A	41	-9.388	69.277	25.179	1.00 65.13	A

Figure 11F

									1		
ATOM	352	N	ALA	A	42	-9.971	67.722	26.679	1.00 67.16	· A	
ATOM	353	CA	ALA	A	42	-11.362	68.150	26.693	1.00 70.08	A	
MOTA	354	CB	ALA		42	-12.252	67.043	27.249	1.00 68.59	A	
ATOM	355	С	ALA		42	-11.461	69.423	27.556	1.00 72.76	. A	
ATOM	356	0	AiA		42	-12.506	69.748	28.123	1.00 73.45	A	
MOTA	357	N	ARG		43	-10.338	70.137	27.642	1.00 75.35	. A	
MOTA	358	CA	ARG		43	-10.202	71.377	28.413	1.00 76.97	A	
ATOM	359	CB	ARG		43	-9.391	71.131	29.705	1.00 77.23	A	
ATOM	360	CG	ARG		43	-10.130	70,250	30.753	1.00 77.63	A	
ATOM	361	œ	ARG		43	-9.265	69.690	31.889	1.00 76.18	. A	
ATOM	362	NE	ARG		43	-10.053	68.919	32.864	1.00 76.19	, A	
ATOM	363	CZ	ARG		43	-10.933	67.967	32.551	1.00 76.17	A	
ATOM	364		ARG		43	-11.153	67.657	31.284	1.00 76.24	A	
ATOM	365		ARG		43	-11.605	67.326	33.507	1.00 77.89	A	
ATOM .	366	С	ARG		43	9.560	72.481	27.570	1.00 79.19	A	
ATOM	367	0	ARG		43.	-10.131	72.882	26.548	1.00 79.42	A	
ATOM	368	N	ILE		44	-8.381	72.970	27.993	1.00 81.42	A	
ATOM	369	CA	ILE		44	-7.646	74.059	27.276	1.00 84.32	A	
ATOM	370	CB	ILE	A	44	-6.073	73.998 74.824	27.495 26.419	1.00 84.97	. A	
MOTA	371	.CG2	ILE	Α.	44	-5.292 -5.728	74.612	28.829	1.00 85.80	. A	
ATOM	372	CG1	ILE		44	-6.344	76.011	29.055	1.00 85.32	. A	
ATOM ATOM	373 374	CDI	ILE		44	-7.908	73.987	25.790	1.00 86.80	A	
ATOM	375	0	ILE		44	-8.577	74.829	25.234	1.00 87.60	A	
ATOM	376	N	LEU		45	-7.318	73.007	25.145	1.00 87.00	A	
ATOM	377	CA	LEU		45	-7.541	72.910	23.737	1.00 88.13	A	
ATOM	378	CB		A	45	-6.257	72.509	23.009	1.00 88.79	A	
ATOM	379	CG	LEU	A	45	-5.940	73.339	21.770	1.00 90.46	A	
ATOM	380			A	45	-7.147	73.370	20.837	1.00 91.58	A	
	381		LEU		45	-5.596	74.779	22.173	1.00 90.84	A	
ATOM	382	C	LEU		45	-8.656	71.944	23.376	1.00 88.30	A	
ATOM	383	ō	LEU		45	-9.507	71.665	24.291	1.00 87.82	A	
ATOM	384	NT		A	45	-8.614	71.561	22.151	1.00 88.77	A	
ATOM	385	CA	ACE	В	0	29.175	18.175	21.874	1.00 35.90	В	
ATOM	386	C	ACE	В	0	27.867	18.849	22.146	1.00 36.69	В	
ATOM	387	0		В	0	27.836	20.078	22.299	1.00 33.24	В	
ATOM	388	N	ARG	В	1	26.771	18.065	22.218	1.00 32.69	В	
ATOM	389	CA	ARG	В	1	25.440	18.590	22.450	1.00 34.24	B.	
ATOM	390	CB	ARG	В	1	24.436	17.446	22.644	1.00 33.49	В	
ATOM	391	CG	ARG	В	1	22.976	17.878	22.651	1.00 32.92	В	
ATOM	392	CD	ARG	В	1	22.436	18.177	21.260	1.00 34.95	В	
ATOM	393	NE	ARG	В	1	22.366	16.972	20.443	1.00 38.88	В	
ATOM	394	CZ	ARG	В	1	21.548	15.952	20.706	1.00 42.79	В	
ATOM	395	NH1	ARG	В	1	20.740	16.012	21.765	1.00 44.66	B	
ATOM	396	NH2	ARG	В	1	21.550	14.868	19.943	1.00 39.72	B	
ATOM	397	С	ARG	В	1	25.424	19.498	23.685	1.00 35.96	В	
ATOM	398	0	ARG	В	1	24.920	20.617	23.628	1.00 36.55	B	
MOTA	399	N	MET	В	2	26.008	19.009	24.779	1.00 39.89	В	
ATOM	400	CA	MET	В	2	26.077	19.769	26.022	1.00 43.08	В	
ATOM	401	CB	MET	В.	. 2	27.113	19.163	26.972	1.00 43.87	В	
ATOM	402	CG	MET	В	2	26.728	17.847	27.623	1.00 46.86	В	
ATOM	403	SD	MET	В	2	25.304	18.010	28.700	1.00 52.01	В	
MOTA	404	CE	MET	В	2	24.024	18.375	27.524	1.00 52.70	В	
ATOM	405	С	MET	В	2	26.440	21.219	25.789	1.00 45.76	В	
MOTA	406	0	MET	В	2	25.723	22.121	26.212	1.00 44.09	3	
ATOM	407	N	LYS	3	3	27.570	21.414	25.125	1.00 47.94	В	
ATOM	408	CA	LYS	В	3	28.082	22.736	24.820	1.00 52.42	В -	
ATOM	409	CB	LYS	В	3	29.455	22.565	24.151	1.00 54.64	. В	
ATOM	410	CG	LYS	B	3	30.552	23.540	24.595	1.00 58.36	Э.	
ATOM	411	CD	LYS	В	3	30.382	24.937	24.030 ·	1.00 60.17	В	

Figure 11G

ATOM	412	CE	LYS		3	31.618	25.777	24.321	1.00 62.06	В
MOTA	413	NZ	LYS		3	31.561	27.140	23.704	1.00 63.71	В
ATOM	414	С	LYS	Ε :	3	27.095	23.479	23.907	1.00 52.65	В
ATOM	415	0	LYS	в :	3	26.858	24.571	24.092	1.00 52.44	В
ATOM	415	Ŋ	GLN	3	4	26.517	22.774	22.934	1.00 52.13	В
ATOM	417	CA	GLN	В .	4	25.549	23.387	22.032	1.00 54.04	В
ATOM	418	CB	GLN	в .	4	24.930	22.330	21.105	1.00 57.72	B
ATOM .	419	CG	GLN	в .	1	25.792	21.880	19.925	1.00 60.44	В
ATOM	420	CD	GLN	3 4	4	25.855	22.923	18.816	1.00 62.71	В
ATOM	421	OE1	GLN	в .	1	26.404	24.017	18.997	1.00 64.51	В
ATOM	422	NE2	GLN		1	25.276	22.592	17.661	1.00 62.62	В
ATOM	423	С	GLN		1	24.441	24.062	22.836	1.00 52.63	В
ATOM	424	ō	GLN		1	24.013	25.162	22.518	1.00 53.56	В
ATOM	425	N	ILE		5	23.982	23.379	23.878	1.00 52.62	В
ATOM	426	CA	ILE			22.929	23.880	24.758	1.00 52.43	В
ATOM	427	CB	ILE		5	22.443	22.766	25.721	1.00 51.17	В
ATOM				В 9		21.412	23.329	26.691	1.00 52.10	B
	428	CG2				21.412	21.592	24.917		
ATOM	429	CG1							1.00 52.55	. В
MOTA	430	CD1		В 5		21.496	20.363	25.754	1.00 53.47	В
ATOM	431	C		В 5		23.452	25.043	25.600	1.00 53.54	В
MOTA	432	0		В 5		22.743	26.013	25.849	1.00 52.58	В
ATOM	433	N	GLU			24.701	24.932	26.036	1.00 55.54	₿
ATOM	434	CA	GLU			25.309	25.970	26.850	1.00 56.11	В
ATOM	435	CB	GLU			26.637	25.477	27.437	1.00 53.75	В
ATOM	436	CG		В 6		26.487	24.157	28.171	1.00 53.07	В
ATOM	437	CD	GLU	В 6	5	27.729	23.735	28.939	1.00 50.56	В
ATOM	438	OE1	GLU	B , 6		28.816	23.611	28.329	1.00 49.24	В
ATOM	439	OE2	GLU	в 6	;	27.604	23.516	30.159	1.00 47.31	В
ATOM	440	С	GLU	в 6	,	25.522	27.217	26.009	1.00 57.04	B
ATOM	441	0	GLU	B 6	i	25.418	28.335	26.515	1.00 58.94	В
ATOM	442	N	ASP	B 7		25.811	27.031	24.725	1.00 57.18	В
ATOM	443	CA	ASP	B 7		26.003	28.179	23.848	1.00 58.51	B
ATOM	444	CB	ASP	в 7		26.681	27.772	22.536	1.00 59.88	·B
ATOM	445	CG	ASP	B 7		28.121	27.339	22.732	1.00 62.42	В
ATOM	446	OD1	ASP	B 7		28.827	27.979	23.542	1.00 62.53	B
ATOM	447	OD2		в 7		28.559	26.382	22.056	1.00 66.19	В
ATOM	448	C		в 7		24.668	28.858	23.543	1.00 58.25	В
ATOM	449	ō		в 7		24.524	30.070	23.314	1.00 56.00	В
ATOM	450	N		в 8		23.591	28.069	23.547	1.00 57.96	В
ATOM	451	CA		3 8		22.240	28.563	23.276	1.00 57.58	В
ATOM	452	CB		B 8		21.331	27.405	22.838	1.00 57.99	B
ATOM	453	CG		в 8		19.911	27.844	22.484	1.00 60.08	B
ATOM	454	CD		B 8		19.915	28.785	21.280	1.00 60.12	B
ATOM	455	CE		B . 8		18.697	29.725	21.268	1.00 60.76	В
ATOM	456	NZ		B 8		17.371	29.062	21.146	1.00 58.46	В
ATOM	457	C		B 8		21.653	29.248	24.517	1.00 56.86	В
				в 8		20.832	30.166	24.317		
ATOM	458	0							1.00 53.70	В
ATOM	459	N				22.077	28.790	25.689	1.00 57.87	В
ATOM	460	CA				21.621	29.368	26.947	1.00 59.31	В
ATOM	461	CB		B 9		22.073	28.517	28.161	1.00 57.40	В
ATOM	462	CG2		B 9		21.788	29.270	29.459	1.00 57.21	. В
ATOM	463		ILE			21.361	27.165	28.154	1.00 56.21	В
ATOM	464		ILE			21.885	26.199	29.212	1.00 54.49	В
MOTA	465	С		B 9		22.216	30.770	27.093	1.00 60.74	₿
ATOM	466	0	ILE	B 9		21.565	31.682	27.608	1.00 61.51	. В
ATOM	467	N		B 10		23.456	30.923	26.633	1.00 61.69	В
MOTA	468	CA	GLU	B 10		24.170	32.198	26.691	1.00 63.76	B
ATOM	469	CB	GLU	B 10		25.629	32.000	26.279	1.00 63.63	B
MOTA	470	CG	GLU	3 10		26.456	33.275	26.254	1.00 65.58	В
ATOM	471	CD	GLU	B 10		27.854	33.054	25.707	1.00 66.48	В

Figure 11H

ATOM	472	OE1	GLU B	10	27,979	32.751	24.499	1.00 67.38		В
ATOM	473	OE2		10	28.824	33.173	26.485	1.00 66.28		В
ATOM	474	c	GLU B	10	23.515	33.211	25.757	1.00 65.16		В
ATOM	475	ō	GLU B	10	23.261	34.351	26.141	1.00 65.81		В
ATOM	476	N	GLU B	11	23.255	32.785	24.524	1.00 66.64		В
ATOM	477	CA	GLU B	11	22.617	33.637	23.529	1.00 67.59		В
		CB		11	22.348	32.832	22.252	1.00 68.72		В
ATOM	478	-	GLU B							-
MOTA	479	CG	GLU B	11	21.735	33.636	21.117	1.00 72.88		В
ATOM	480	CD	GLU B	11	22.556	34.864	20.767	1.00 74.80		В
ATOM	481	OE1		11	23.775	34.717	20.526	1.00 75.81		В
ATOM	482	OE2		11	21.978	35.975	20.731	1.00 74.99		В
ATOM	483	C	GLU B	11	21.307	34.197	24.098	1.00 67.17		В
ATOM	484	0	GLU B	11	20.998	35.381	23.918	1.00 68.06		В
ATOM	485	N	ILE B	12	20.541	33.348	24.784	1.00 64.61		В.
MOTA	486	CA	ILE B	12	19.288	33.790	25.389	1.00 61.65		В
MOTA	487	CB	ILE B	12	18.458	32.600	25.926	1.00 62.84	1	В
ATOM	488	CG2	ILE B	12	17.416	33.094	26.940	1.00 62.63	1	В
ATOM	489	CGl	ILE B	12	17.799	31.864	24.750	1.00 62.13	1	В
ATOM	490	CD1	ILE B	12	16.910	30.698	25.156	1.00 61.39	,	В
ATOM	491	C	ILE B	12	19.553	34.776	26.522	1.00 58.17	1	В
ATOM	492	0	ILE B	12	19.010	35.881	26.523	1.00 55.05	1	В
ATOM	493	N	GLU B	13	20.388	34.384	27.479	1.00 55.87	1	В
ATOM	494	CA	GLU B	13	20.710	35.268	28.600	1.00 54.71	I	В
ATOM	495	CB	GLU B	13	21.817	34.669	29.477	1.00 50.19	1	В
MOTA	496	CG	GLU B	13	21.447	33.331	30.109	1.00 49.30	1	3
ATOM	497	CD	GLU B	13	22.577	32.729	30.933	1.00 49.10	1	3
ATOM	498		GLU B	13	23.741	32.765	30.472	1.00 50.79	I	3
ATOM	499	OE2		13	22.304	32.194	32.027	1.00 47.00	I	3
ATOM	500	С	GLU B	13	21.166	36.512	28.047	1.00 55.57	I	3
ATOM	501	0	GLU B	13	20.790	37.667	28.557	1.00 56.33	F	3
ATOM	502	N	SER B	14	21.950	36.559	26.977	1.00 56.02	I	3
ATOM	503	CA	SER B	14	22.468	37.763	26.350	1.00 55.71	I	
ATOM	504	CB	SER B	14	23.488	37.389	25.278	1.00 54.62	I	
ATOM	505	OG	SER B	14	23.968	38.550	24.629	1.00 56.74	I	
ATOM	506	Ċ	SER B	14	21.366	38.624	25.736	1.00 55.96	Ξ	
ATOM	507	ō	SER B	14	21.469	39.854	25.696	1.00 54.91	E	
ATOM	508	N	LYS B	15	20.310	37.979	25.263	1.00 55.94	E	
ATOM	509	CA	LYS B	15	19.208	38.704	24.650	1.00 56.72	E	
ATOM	510	CB	LYS B	15	18.454	37.779	23.693	1.00 55.67	E	
ATOM	511	CG	LYS B	15	17.494	38.484	22.772	1.00 58.33		
ATOM	512	CD	LYS B	15	17.000	37.527	21.705	1.00 59.89	Ē	
ATOM	513	CE	LYS B	15	16.440	38.282	20.518	1.00 60.44	E	
ATOM	514	NZ	LYS B	15	16.020	37.375	19.412	1.00 63.67	E	
ATOM	515	C	LYS B	15	18.282	39.207	25.748	1.00 56.31	Ē	
ATOM	516	0	LYS B	15	17.716	40.296	25.661	1.00 56.65	Ē	
ATOM	517	N.	GLN B	16	18.146	38.403	26.791	1.00 56.76	E	
ATOM	518	CA	GLN B	16	17.293	38.748	27.911	1.00 57.28	E	-
ATOM	519	CB	GLN B	16	17.306	37.604	28.923	1.00 56.94	E	
ATOM	520	CG	GLN B	16	16.000	37.394	29.652	1.00 55.90	E	
ATOM	521	CD	GLN B	16	15.908	36.017	30.300	1.00 56.24	E	
					16.613	35.722	31.263	1.00 57.78	E	
ATOM	522	OE1	GLN B	16	15.044	35.722	29.760	1.00 55.69	E	
ATOM	523	NE2		16					E	
ATOM	524	С	GLN B	16	17.825	40.040	28.528	1.00 58.82	E	
ATOM	525	0	GLN B	16	17.049	40.929	28.905	1.00 59.68	Ξ	
ATOM	526	N	LYS B	17	19.148	40.163	28.621	1.00 59.44		
ATOM	527	CA	LYS B	17	19.711	41.379	29.189	1.00 59.84	E	
ATOM	528	CB	LYS B	17	21.228	41.275	29.386	1.00 60.80		
ATOM	529	CG	LYS B	17	21.740	42.343	30.356	1.00 64.52	12	
ATOM	530	CD	LYS B	17	23.250	42.325	30.576	1.00 65.30	2	
ATOM	531	CE	LYS B	17	24.008	42.784	29.344	1.00 67.22	E	

Figure 111

```
ATOM
           532
                     LYS B
                                       25.465
                                                42.963
                                                        29.525
                                                                 1.00 67.09
  ATOM
           533
                C
                     LYS B
                             17
                                       19.389
                                                42.522
                                                        28.230
                                                                 1.00
  ATOM
           534
                0
                     LYS B
                             17
                                      19.088
                                               43.634
42.233
                                                        28.656
                                                                 1.00
                                                                                   В
  ATOM
           535
                N
                     LYS B
                             18
                                       19.433
                                                        26.931
                                                                 1.00
                                                                      56.38
                                                                                   В
  ATOM
           536
                CA
                     LYS B
                             18
                                      19.128
                                               43.248
                                                        25.931
                                                                 1.00 58.35
                                                                                   В
  ATOM
           537
                CB
                     LYS B
                                      19.247
                                               42.675
                                                        24.511
                                                                 1.00
                                                                      59.38
                                                                                   В
  ATOM
           538
                ·CG
                     LYS B
                             18
                                      20.617
                                               42.083
                                                        24.130-
                                                                 1.00 61.47
                                                                                   В
  ATOM
           539
                CD
                     LYS B
                             18
                                      21.768
                                               43.111
                                                        24.099
                                                                 1.00 61.91
                                                                                   В
  ATOM
           540
                CE
                     LYS B
                             18
                                      22.034
                                               43.761
                                                        25.461
                                                                 1.00 63.50
                                                                                   В
  АТОМ
                                      23.248
           541
                NZ
                     LYS B
                             18
                                               44.620
                                                        25.423
                                                                 1.00 63.66
                                                                                   В
  ATOM
           542
                С
                     LYS
                         В
                             18
                                               43.761
                                                        26.163
                                                                 1.00 58.27
                                                                                   В
  ATOM
          543
                0
                                      17.475
                     LYS B
                             18
                                               44.969
                                                        26.254
                                                                 1.00 58.82
                                                                                   В
  ATOM
          544
                N
                     ILE B
                             19
                                      16.757
                                               42.835
                                                        26.268
                                                                 1.00-56.89
                                                                                   В
 ATOM
          545
                CA
                     ILE B
                            19
                                      15.356
                                               43.189
                                                        26.488
                                                                 1.00 53.76
                                                                                   В
 ATOM
          546
                CB
                    ILE B
                            19
                                      14.455
                                               41.931
                                                       26.488
                                                                1.00 53.33
                                                                                   В
 MOTA
          547
                CG2
                    ILE B
                            19
                                      13.057
                                               42.286
                                                       26.976
                                                                1.00 52.66
                                                                                   В
 ATOM
          548
                CG1
                    ILE B
                            19
                                      14.416
                                               41.322
                                                       25.081
                                                                1.00 52.79
                                                                                   В
 ATOM
          549
                CD1 ILE B
                            19
                                      13.543
                                               40.069
                                                       24.970
                                                                1.00 54.45
                                                                                   В
 ATOM
          550
                C
                    ILE B
                            19
                                      15.117
                                               43.961
                                                       27.786
                                                                .1.00 52.88
                                                                                   В
 ATOM
          551
                0
                    ILE B
                            19
                                     14.327
                                               44.897
                                                       27.809
                                                                1.00 51.74
                                                                                   В
 ATOM
          552
                N
                    GLU B
                            20
                                     15.781
                                               43.565
                                                       28.869
                                                                1.00 51.04
                                                                                  В
 ATOM
                CA
                    GLU B
                            20
                                     15.601
                                               44.267
                                                       30.128
                                                                1.00 50.08
                                                                                  В
 ATOM
          554
                СВ
                    GLU B
                            20
                                     16.403
                                              43.613
                                                       31.253
                                                                1.00 49.90
                                                                                  В
 ATOM
          555
                CG
                    GLU B
                            20
                                     15.969
                                              42.207
                                                       31.584
                                                                1.00 54.19
 ATOM
          556
               CD
                    GLU B
                            20
                                     16.761
                                                       32.736
                                              41.620
                                                                1.00 55.98
                                                                                  В
 ATOM
          557
               OE1
                   GLU B
                            20
                                     18.010
                                              41.568
                                                       32.641
                                                                1.00 53.23
 ATOM
          558
               OE2
                   GLU B
                            20
                                     16.127
                                              41.215
                                                       33.735
                                                                1.00 56.20
 ATOM
          559
               C
                    GLU B
                            20
                                     16.053
                                              45.706
                                                       29.965
                                                                1.00 49.26
 ATOM
               0
          560
                    GLU B
                           20
21
                                     15.479
                                              46.611
                                                       30.561
                                                                1.00 48.88
                                                                                  В
 ATOM
          561
               N
                    ASN B
                                     17.093
                                              45.912
                                                       29.163
                                                                1.00 49.15
 ATOM
               CA
          562
                   ASN B
                           21
                                     17.596
                                              47.256
                                                      28.930
                                                               1.00 49.99
                                                                                  В
ATOM
          563
               CB
                   ASN B
                           21
                                     18.885
                                              47.229
                                                      28.098
                                                               1.00 51.35
MCTA
         564
               CG
                   ASN B
                           21
21
                                     20.054
                                              46.576
                                                      28.834
                                                               1.00 54.79
                                                                                  В
ATOM
         565
               OD1
                   ASN B
                                     20.421
                                              46.978
                                                      29.943
                                                               1.00 55.96
ATOM
         566
               ND2
                   ASN B
                           21
                                     20.656
                                              45.572
                                                      28.205
                                                               1.00 57.15
                                                                                  В
ATOM
         567
               \mathsf{C}
                   ASN B
                           21
                                     16.537
                                              48.078
                                                      28.202
                                                               1.00 49.83
ATOM
               ō
         568
                   ASN B
                           21
                                    16.249
                                                      28.591
                                              49.209
                                                               1.00 50.14
ATOM
         569
               Ν
                   GLU B
                           22
                                    15.957
                                              47.497
                                                      27.153
                                                               1.00 47.34
ATOM
         570
               CA
                           22
                   GLU B
                                    14.942
                                             48.160
                                                      26.354
                                                               1.00 44.99
                                                                                 В
ATOM
         571
               CB
                   GLU B
                           22
                                    14.534
                                             47.272
                                                      25.174
                                                               1.00 44.99
                                                                                 В
ATOM
         572
               CG
                   GLU B
                           22
                                    13.703
                                             47.990
                                                      24.116
                                                               1.00 51.85
                                                                                 В
         573
ATOM
               CD
                   GLU B
                           22
                                    14.377
                                             49.268
                                                               1.00 54.71
1.00 55.60
                                                      23.621
                                                                                 В
ATOM
         574
              OE1
                   GLU B
                           22
                                    15.543
                                             49.191
                                                      23.182
                                                                                 В
ATOM
         575
              OE2
                   GLU B
                           22
                                    13.743
                                             50.350
                                                      23.673
                                                               1.00 57.01
                                                                                 В
ATOM
         576
              C,
                   GLU B
                           22
                                    13.710
                                             48.521
                                                      27.183
                                                               1.00 44.17
         577
                                                                                 В
ATOM
              0
                   GLU B
                           22
                                    13.044
                                                      26.916
                                             49.527
                                                               1.00 45.50
                                                                                 В
ATOM
         578
              N
                   ILE B
                           23
                                    13.386
                                             47.693
                                                      28.169
                                                               1.00 42.28
                                                                                 В
ATOM
         579
              ·CA
                   ILE B
                           23
                                    12.241
                                             47.977
                                                      29.024
                                                               1.00 40.61
                                                                                 В
ATOM
         580
              CB
                   ILE B
                          23
                                    11.801
                                             46.724
                                                      29.809
                                                               1.00 38.57
                                                                                 В
ATOM
         581
              CG2
                   ILE B
                           23
                                    10.836
                                             47.096
                                                     30.925
                                                              1.00 37.31
                                                                                 В
ATOM
         582
              CG1
                  ILE B
                                    11.138
                                             45.733
                                                     28.850
                                                               1.00 38.28
                                                                                 В
ATOM
        583
              CD1
                   ILE B
                           23
                                    10.634
                                             44.436
                                                     29.530
                                                              1.00 38.32
                                                                                 В
ATOM
                                    12.626
11.793
        584
              C
                   ILE B
                          23
                                             49.108
                                                     29.974
                                                              1.00
                                                                    41.50
                                                                                 B
ATCM
        585
              0
                   ILE B
                          23
                                             49.926
                                                     30.349
                                                              1.00 41.54
                                                                                 В
ATOM
        586
              N
                   ALA B
                          24
                                    13.898
                                             49.170
                                                     30.348
                                                              1.00 40.42
                                                                                 В
ATOM
        587
              CA
                  ALA
                          24
                                    14.349
                                             50.240
                                                     31.224
                                                              1.00 38.49
                                                                                 В
ATOM
        588
              СВ
                   ALA E
                          24
                                    15.811
                                             50.059
                                                     31:578
                                                              1.00
                                                                                3
ATOM
        589
              C
                  ALA B
                          24
                                    14.147
                                             51.562
                                                     30.490
                                                              1.00
                                                                                3
ATOM
        590
              0
                  ALA B
                          24
                                    13.674
                                            52.528
                                                     31.078
                                                              1.00
                                                                    38.39
                                                                                В
ATOM
        591
              N
                  ARG
                                   14.498
                                            51.591
                                                     29.204
                                                              1.00 36.47
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Figure 11J

ATOM 616 NZ LYS B 27											
ATOM 593 CB ARG B 25				A Al	RG :	B 25	14.35	54 52.79	96 28.39	4 1 00 38 10	ם ו
ATOM 594 CG ARG B 25 16.609 52.668 27.195 1.00 46.74 ATOM 595 CD ARG B 25 17.315 52.949 22.879 1.00 56.83 ATOM 596 NE ARG B 25 17.884 50.666 25.152 1.00 39.56 ATOM 597 CZ ARG B 25 17.894 50.666 25.152 1.00 39.56 ATOM 598 NH1 ARG B 25 17.792 49.696 24.257 1.00 59.81 ATOM 599 NH2 ARG B 25 17.792 49.696 24.257 1.00 59.81 ATOM 600 C ARG B 25 12.901 51.185 28.158 1.00 36.71 ATOM 601 O ARG B 25 12.901 51.185 28.158 1.00 36.74 ATOM 602 N ILE B 26 12.051 52.197 7.942 1.00 36.54 ATOM 603 CA ILE B 26 12.051 52.197 7.942 1.00 36.54 ATOM 603 CA ILE B 26 12.051 52.197 7.942 1.00 36.54 ATOM 605 CG2 ILE B 26 10.642 52.454 27.733 1.00 34.16 ATOM 606 CG1 ILE B 26 10.435 50.722 25.985 1.00 34.16 ATOM 607 CD1 ILE B 26 10.435 50.722 25.985 1.00 34.01 ATOM 608 CG ILE B 26 10.435 50.722 25.985 1.00 34.40 ATOM 608 CG ILE B 26 9.317 54.053 28.956 1.00 31.45 ATOM 609 N ILE B 26 9.317 54.053 28.956 1.00 34.37 ATOM 601 N LYS B 27 10.366 53.059 29.005 1.00 34.32 ATOM 610 N LYS B 27 10.366 52.005 32.544 1.00 35.31 ATOM 613 CG LYS B 27 10.366 52.005 32.544 1.00 35.31 ATOM 614 CD LYS B 27 10.366 52.005 32.544 1.00 36.43 ATOM 615 CE LYS B 27 10.366 52.005 32.544 1.00 36.43 ATOM 616 NZ LYS B 27 10.366 52.005 32.544 1.00 35.31 ATOM 617 C LYS B 27 10.366 52.005 32.544 1.00 36.43 ATOM 618 NZ LYS B 27 10.366 52.005 32.544 1.00 36.43 ATOM 619 N LYS B 27 10.366 55.140 33.347 1.00 44.66 ATOM 610 NZ LYS B 27 10.366 55.140 33.347 1.00 44.66 ATOM 610 NZ LYS B 27 10.366 55.140 33.347 1.00 44.66 ATOM 612 CB LYS B 27 10.366 55.140 33.347 1.00 35.31 ATOM 614 CD LYS B 27 10.366 55.140 33.347 1.00 36.82 ATOM 616 NZ LYS B 27 10.366 55.140 33.347 1.00 36.82 ATOM 617 C LYS B 27 10.366 55.140 33.347 1.00 36.82 ATOM 618 O LYS B 27 10.366 55.140 33.347 1.00 36.82 ATOM 619 N LYS B 28 11.599 54.670 31.266 1.00 36.91 ATOM 610 NZ LYS B 28 13.667 56.017 30.988 1.00 42.60 ATOM 620 C LYS B 28 13.667 56.017 30.988 1.00 42.60 ATOM 630 C B LEU B 29 9.958 59.581 26.20 1.00 37.70 ATOM 631 C LEU B 29 9.467 53.887 34.421 1.00 36.49 ATOM 634 C LEU B 29 9.455 53.887 31.240 1.00 36				B Al	RG I	B 25	15.08	36 52.64			
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ATOM 632 CD1 LEU B 29 9.958 59.581 26.260 1.00 36.39 1 ATOM 633 CD2 LEU B 29 9.441 57.641 24.744 1.00 35.00 1 ATOM 634 C LEU B 29 9.103 57.912 29.047 1.00 35.09 ATOM 635 O LEU B 29 8.568 59.015 29.095 1.00 34.76 1 ATOM 636 N LEU B 30 8.512 56.787 29.426 1.00 33.74 1 ATOM 637 CA LEU B 30 7.161 56.746 29.946 1.00 33.74 1 ATOM 638 CB LEU B 30 6.789 55.284 30.181 1.00 32.72 1 ATOM 639 CG LEU B 30 6.789 55.284 30.181 1.00 32.72 1 ATOM 639 CG LEU B 30 6.789 55.284 30.181 1.00 32.72 1 ATOM 640 CD1 LEU B 30 6.789 55.284 30.558 1.00 31.65 1 ATOM 640 CD1 LEU B 30 6.985 57.588 31.213 1.00 31.65 1 ATOM 640 CD1 LEU B 30 6.985 57.588 31.213 1.00 31.65 1 ATOM 640 CD1 LEU B 30 6.985 57.588 31.213 1.00 31.56 1 ATOM 642 C LEU B 30 6.985 57.588 31.213 1.00 31.56 1 ATOM 645 CA GLN B 31 7.860 57.442 32.206 1.00 31.24 1 ATOM 645 CA GLN B 31 7.860 57.442 32.206 1.00 31.24 1 ATOM 645 CA GLN B 31 7.860 57.442 32.206 1.00 33.79 1 ATOM 646 CB GLN B 31 7.860 57.442 32.206 1.00 33.79 1 ATOM 647 CG GLN B 31 10.013 57.729 34.321 1.00 40.81 1 ATOM 648 CD GLN B 31 10.013 57.729 34.321 1.00 40.81 1 ATOM 649 OE1 GLN B 31 10.804 57.648 36.598 1.00 41.97 1 BOTOM 650 NE2 GLN B 31 11.270 55.889 35.258 1.00 41.97 1 BOTOM 650 NE2 GLN B 31 11.270 55.889 35.258 1.00 41.97 1 BOTOM 650 NE2 GLN B 31 11.270 55.889 35.258 1.00 41.97 1 BOTOM 651 CT TO THE TOT TO THE TO									27.071	1.00 36.49	В
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ATOM 645 CA GLN B 31 7.668 58.265 33.398 1.00 33.01 B ATOM 646 CB GLN B 31 8.551 57.801 34.564 1.00 33.79 B ATOM 647 CG GLN B 31 10.013 57.729 34.321 1.00 40.81 B ATOM 648 CD GLN B 31 10.737 57.086 35.491 1.00 44.04 B ATOM 649 OE1 GLN B 31 10.804 57.648 36.598 1.00 42.99 B ATOM 650 NE2 GLN B 31 11.270 55.889 35.258 1.00 41.97 B											B
ATOM 646 CB GLN B 31 8.551 57.801 34.564 1.00 33.79 B ATOM 647 CG GLN B 31 10.013 57.729 34.321 1.00 40.81 B ATOM 648 CD GLN B 31 10.737 57.086 35.491 1.00 44.04 B ATOM 649 OE1 GLN B 31 10.804 57.648 36.598 1.00 43.99 B ATOM 650 NE2 GLN B 31 11.270 55.889 35.258 1.00 41.97 B								58.265			В
ATOM 649 OEI GLN B 31 10.013 57.729 34.321 1.00 40.81 B ATOM 648 CD GLN B 31 10.737 57.086 35.491 1.00 44.04 B ATOM 649 OEI GLN B 31 10.804 57.648 36.598 1.00 43.99 B ATOM 650 NE2 GLN B 31 11.270 55.889 35.258 1.00 41.97 B											В
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ATOM 650 NE2 GLN B 31 11.270 55.889 35.258 1.00 41.97 B											В
DTOM 551 C CIN D 21											₿
7.906 59.734 23.072 1.00 34.12 B											
		331	-	GIIIV	5	J 1	7.906	D9./54	33.072	1.00 34.12	В

Figure 11K

Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion Inventors: Debra M. Eckert, et al.

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ATOM
           652
                0
                     GLN B
                                       7.420 60.636
                                                       33.766
                                                                1.00 30.63
                                                                                  В
  АТОМ
           653
                N
                     LEU B
                                       8.629
                                              59.961
                                                       31.984
                                                                1.00 34.46
                                                                                  В
  ATOM
           654
                CA
                     LEU B
                                       8.935
                                              61.292
                                                       31.523
                                                                1.00 36.10
                                                                                  В
  ATOM
           655
                CB
                     LEU B
                             32
                                      10.070
                                              61.231
                                                       30.504
                                                                1.00 40.01
                                                                                  В
  ATOM
           656
                CG
                     LEU B
                             32
                                     10.340
                                              62.546
                                                       29.775
                                                               1.00 40.15
  ATOM
           657
                CD1
                     LEU
                             32
                                      10.853
                                              63.586
                                                       30.765
                                                                1.00 43.23
                                                                                  В
  ATOM
           658
               · CD2
                     LEU B
                            32
                                     11.354
                                              62.310
                                                       28.668
                                                                1.00 43.00
                                                                                 В
  ATOM
           659
                С
                     LEU B
                            32
                                      7.711
                                                       30.890
                                              51.949
                                                                1.00 36.08
                                                                                 В
  ATOM
           660
                            32
                     LEU B
                                      7.552
                                                       30.964
                                              63.162
                                                                1.00 37.71
                                                                                 В
  ATOM
           661
                N
                     THR B
                            33
                                      6.859
                                              61.149
                                                       30.255
                                                                1.00 32.40
                                                                                 ₿
  ATOM
           662
                CA
                    THR B
                            33
                                                               1.00 31.31
1.00 30.70
                                      5.659
                                              61.679
                                                       29.617
                                                                                 В
  ATOM
           663
                CB
                     THR B
                            33
                                      5.179
                                              60.753
                                                       28.480
                                                                                 В
  ATOM
           664
                0G1
                    THR B
                            33
                                      4.536
                                              59.603
                                                       29.030
                                                               1.00 40.03
                                                                                 В
  ATOM
           665
                CG2
                    THR B
                            33
                                      6.371
                                              60.282
                                                      27.654
                                                               1.00 31.28
                                                                                 В
  ATOM
           666
                С
                    THR B
                            33
                                      4.550
                                              61.845
                                                      30.668
                                                               1.00 30.03
                                                                                 В
 ATOM
           667
                0
                    THR B
                            33
                                      3.739
                                              62.772
                                                      30.585
                                                               1:00 30.10
                                                                                 В
  ATOM
           668
                N
                    VAL B
                            34
                                      4.507
                                              60.933
                                                      31.636
                                                               1.00 27.29
 ATOM
           669
                ÇA
                    VAL B
                            34
                                      3.546
                                              61.010
                                                      32.735
                                                               1.00 25.28
                                                                                 В
 ATOM
          670
                СВ
                    VAL B
                            34
                                      3.695
                                              59.806
                                                               1.00 26.71
1.00 27.25
                                                      33.690
 ATOM
          671
                CG1
                    VAL B
                            34
                                      2.920
                                              60.036
                                                      34.985
                                                                                 В
                    VAL B
 ATOM
          672
               CG2
                            34
                                      3.176
                                                      32.997
                                             58.565
                                                               1.00 23.84
 ATOM
               C
          673
                    VAL B
                                                      33.476
                            34
                                      3.822
                                             62.310
                                                               1.00 22.65
                                                                                В
 ATOM
               0
          674
                    VAL B
                                                      33.763
                            34
                                      2.899
                                             63.064
                                                              1.00 21.36
                                                                                В
 ATOM
               N
          675
                    TRP B
                            35
                                      5.100
                                             62.580
                                                               1.00 22.24
                                                                                В
 ATOM
          676
               CA
                    TRP B
                            35
                                      5.502
                                             63.828
                                                      34.414
                                                              1.00 20.87
                                                                                В
 ATOM
          677
               CB
                    TRP B
                            35
                                     7.016
                                                      34.653
                                             63.843
                                                              1.00 23.71
 ATOM
          678
               CG
                    TRP B
                            35
                                      7.523
                                             65.040
                                                      35.434
                                                              1.00 26.08
 ATOM
               CD2 TRP B
          679
                            35
                                     7.013
                                             65.551
                                                      36.681
                                                              1.00 25.13
                                                                                В
 ATOM
          680
               CE2
                   TRP B
                           35
                                     7.767
                                             66.698
                                                     37.003
37.547
                                                              1.00 28.35
                                                                                В
               CE3 TRP B
 ATOM
          681
                           35
                                     5.985
                                             65.143
                                                              1.00 24.83
                                                                                В
 ATOM
          682
               CD1 TRP B
                           35
                                     8.540
                                             65.880
                                                      35.074
                                                              1.00 25.67
                                                                                В
 ATOM
          683
               NE1 TRP B
                           35
                                     8.692
                                             66.877
                                                     36.006
                                                              1.00 27.74
                                                                                В
 ATOM
          684
               CZ2
                   TRP B
                           35
                                     7.532
                                             67.455
                                                     38.165
                                                              1.00 28.38
                                                                                В
 ATOM
         685
               CZ3 TRP B
                           35
                                     5.749
                                             65.889
                                                     38.699
                                                              1.00 23.47
                                                                                В
 ATOM
         686
               CH2
                   TRP B
                           35
                                            67.034
                                     6.516
                                                     38.999
                                                              1.00 28.31
                                                                                В
 ATOM
         687
               ¢
                   TRP B
                           35
                                     5.121
                                            65.039
                                                     33.564
                                                              1.00 24.26
                                                                                В
ATOM
         688
               0
                   TRP B
                           35
                                     4.695
                                            66.063
                                                     34.088
                                                              1.00 23.94
                                                                                В
ATOM
         689
              N
                   GLY B
                                     5.308
                                            64.927
                                                     32.247
                                                              1.00
                                                                   25.59
                                                                                В
ATOM
         690
              CA
                   GLY B
                           36
                                            66.013
                                     4.961
                                                     31.348
                                                              1.00 23.22
                                                                                В
ATOM
         691
              С
                   GLY B
                          36
                                     3.479
                                                     31.343
                                                              1.00 25.72
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ATOM
         692
              0
                   GLY B
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                                     3.138
                                            67.539
                                                     31.352
                                                             1.00 28.94
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ATOM
         693
              N
                   ILE B
                           37
                                     2.510
                                            65.356
                                                             1.00 27.20
                                                     31.311
                                                                               В
ATOM
         694
              CA
                   ILE B
                           37
                                     1.160
                                            65.560
                                                     31.315
                                                             1.00 24.67
                                                                               В
ATOM
         695
              CB
                   ILE B
                           37
                                    0.429
                                            64.223
                                                    31.230
                                                             1.00 24.72
                                                                               B
ATOM
         696
              CG2
                  ILE B
                           37
                                   -1.085
                                            64.410
                                                    31.416
                                                             1.00 29.15
                                                                               В
ATOM
         697
              CG1 ILE B
                           37
                                    0.700
                                            63.581
                                                    29.879
                                                             1.00
                                                                   22.40
                                                                               В
ATOM
         698
              CD1
                  ILE B
                           37
                                    0.023
                                            62.237
                                                    29.714
                                                             1.00 24.46
                                                                               В
ATOM
         699
                  ILE B
                          37
                                    0.734
                                            66.295
                                                    32.579
                                                             1.00 25.86
                                                                               В
ATOM
         700
              0
                  ILE B
                          37
                                   -0.019
                                            67.255
                                                    32.517
                                                             1.00 25.23
                                                                               В
ATOM
         701
              N
                  LYS B
                                    1.242
                                           65.840
                                                    33.722
                                                             1.00 26.17
                                                                               B
ATOM
         702
              CA
                  LYS B
                          38
                                    0.967
                                            66.449
                                                    35.020
                                                             1.00 22.96
                                                                               В
ATOM
         703
              CB
                  LYS B
                          38
                                    1.656
                                            65.652
                                                    36.130
                                                             1.00 22.07
                                                                               В
ATOM
         704
              CG
                  LYS B
                          38
                                    0.953
                                           64.410
                                                    36.522
                                                             1.00 25.14
                                                                               В
ATOM
        705
              CD
                  LYS 3
                          38
                                           64.727
63.468
                                   -0.225
                                                    37.423
                                                             1.00 28.48
1.00 28.77
                                                                               В
ATOM
        706
              CE
                  LYS B
                          38
                                   -1.014
                                                    37.617
                                                                               В
ATOM
        707
              NZ
                  LYS B
                          38
                                   -1.331
                                           62.953
                                                    36.269
                                                             1.00 34.06
ATOM
        708
              С
                  LYS B
                          38
                                    1.458
                                           67.877
                                                    35.102
                                                             1.00 23.87
ATOM
        709
              0
                  LYS B
                          38
                                    0.770
                                                    35.640
                                                             1.00 20.93
                                           68.736
ATOM
        710
              N
                  GLN B
                          39
                                    2.662
                                           68.140
                                                    34.593
ATOM
                  GLN B
                                    3.189
                                                    34.682
                                           69.493
                                                            1.00 30.76
```

Figure 11L

ATOM	71	2 C	e or	N I	3 39	4.62	9 69.58	2 24 40		
ATOM	71			N E		5.43				-
ATOM	71			NE		4.82				
ATOM	71			NE		4.88				
ATOM	71	6. N		N E		4.22				_
ATOM	71	7 C		NΞ		2.34				
ATOM	718	8 0	GL	NE	3.9	2.12				_
MOTA	719	9 N	LE	UE	4.0	1.89				_
MOTA	720) C2	LE	υĖ	40	1.06				-
ATOM	721	l CE	3 LE	U B	40	0.87				
ATOM	722		LE	U B	40	-0.12				
ATOM	723)1 LE	U B	40	0.17				
ATOM	724			U B	40	-0.058				
ATOM	725		LE	UΒ	40	-0.289	70.94			_
MOTA	726			UВ	40	-0.874	72.010			
ATOM	727			N B	41	-0.768	69.964	33.215		
ATOM	728			ИΒ	41	-2.046	70.063			
. ATOM	729			N B	41	-2369	68.718	34.517		
ATOM	730			N B	41	-3.833	68.459	34.735		
ATOM	731			N B	41	-4.070	67.139	35.420	1.00 54.0	
ATOM	732				41	-3.517			1.00 55.43	
ATOM	733				41	-4.908			1.00 54.90	
ATOM	734		GL1		41	-2.039			1.00 39.95	
MOTA	735	0	GL1		41	-2.988			1.00 39.23	
ATOM	736	N	ALA		42	-0.972			1.00 39.05	В
ATOM	737	CA	ALA		42	-0.845	72.188		1.00 38.56	B
ATOM ATOM	738 739		ALA		42	0.345	71.852		1.00 34.14	В
ATOM	740	C	ALA		42	-0.647	73.566		1.00 40.18	
ATOM	741	O N	ALA ARG		42	-1.139	74.560	36.765	1.00 41.44	
ATOM	742	CA	ARG		43 43	0.078	73.634	35.118	1.00 41.82	
ATOM	743	CB	ARG		43	0.340	74.910	34.476	1.00 43.71	
ATOM	744	CG	ARG		43	1.242	74.713	33.260	1.00 47.26	
ATOM	745	CD	ARG		43	2.582	75.997 75.677	32.592	1.00 51.08	
ATOM	746	NE	ARG		43	3.778	74.947	31.401	1.00 54.95	В
ATOM	747	CZ	ARG		43	4.819	75.499	31.813 32.428	1.00 57.04	В
ATOM	748	NH1			43	4.816	76.794	32.703	1.00 56.95	В
ATOM	749	NH2			43	5.858	74.753	32.781	1.00 55.89	В
ATOM	750	C	ARG		43	-0.987	75.521	34.048	1.00 57.00 1.00 42.38	В
MOTA	751	0	ARG		43	-1.308	76.657		1.00 42.38	В
ATOM	752	N ·	ILE	В	44	-1.756	74.736	33.310	1.00 41.41	. В
ATOM	753	CA	ILE	В	44	-3.059	75.143	32.810	1.00 43.24	B B
MOTA	754	CB	ILE	В	44	-3.634	74.085	31.866	1.00 44.23	B
ATOM	755	CG2	ILE	В	44	-5.083	74.403		1.00 45.04	В
ATOM	756	CG1	ILE		44	-2.778	73.964	30.600	1.00 47.45	В
ATOM	757	CD1	ILE	₽	44	-3.156	72.745	29.719	1.00 49.42	3
MOTA	758	С		В	44	-4.081	75.306	33.935	1.00 42.37	B
ATOM	759	0		В	44	-4.422	76.416	34.332	1.00 42.08	В
ATOM	760	N	LEU	В	45	-4.573	74.162	34.398	1.00 42.20	. в
ATOM	761	CA	LEU		45	-5.564	74.042	35.450	1.00 43.16	В
ATOM	762	CB	LEU		45	-6.041	72.592	35.513.	1.00 46.08	В
ATOM	763	CG	LEU		45	-6.459	72.001	34.162	1.00 47.45	В
ATOM	764		LEU		45	-7.011	70.594	34.357	1.00 47.51	В
MOTA	765		LEU		45	-7.504	72.899	33.521	1.00 48.61	В
ATOM	766	C	LEU		45	-5.016	74.467	36.810	1.00 42.48	В
ATOM ATOM	767 768	0	LEU		45	-5.674	75.260	37.483	1.00 45.15	3
ATOM	768 769	NT	LEU		45	-3.945	73.987	37.206	1.00 45.66	3
ATOM	770	CA C		C	0	15.143	11.286	26.819	1.00 82.49	С
ATOM	771	0	ACE		0	14.956	12.476	27.674	1.00 82.44	С
111 011	, , ,	5	ACE	·	0	13.700	12.858	27.851	1.00 84.06	С

Figure 11M

ATOM 772 N ARG C 15.890 13.103 1 28.220 1.00 82.91 773 MOTA CA ARG C 1 15.663 14.253 29.073 1.00 83.87 ATOM 774 ARG C CB 1 16.156 13.970 30.491 1.00 83.74 С 775 ATOM CG 1 ARG C 15.769 15.065 31.456 1.00 83.47 С ATOM 776 CD ARG C 1 14.340 15.542 31.156 1.00 81.66 С ATOM 777 NE ARG C 1 13.249 14.748 31.726 1.00 81.00 ARG C ATOM 778 CZ 1 13.069 13.434 31.597 1.00 79.16 C ATOM 779 NH1 ARG С 1 13.901 12.678 30.889 1.00 79.80 ATOM 780 NH2 ARG C 1 12.010 12.875 32.168 1.00 79.18 C 1 ATOM 781 С ARG · C 16.282 15.541 28.550 1.00 85.03 ATOM 782 0 ARG C 1 15.975 16.644 29.016 1.00 85.10 C ATOM 783 N MET С 2 17.169 15.394 27.581 1.00 85.40 C C ATOM 784 CA MET C 2 17.778 27.012 16.568 1.00 86.91 ATOM 785 CB MET C 2 19.063 16.215 26.290 1.00 88.20 Ç MOTA 786 CG MET C 2 19.711 17.410 25.653 1.00 89.72 С ATOM 787 SĎ MET 2 21.192 16.917 1.00 94.98 24.823 С ATOM 788 CE MET C 2 16.349 22.111 26.176 1.00 91.53 C ATOM 789 С MET C 2 16.771 17.154 26.036 1.00 87.44 ATOM 790 0 MET C 2 16.699 18.368 25.872 1.00 89.05 C ATOM 791 N LYS C 3 16.001 16.278 25.391 1.00 85.66 С ATOM 792 3 CA LYS C 14.973 16.712 24.444 1.00 83.09 C MOTA 793 ÇВ 3 14.033 LYS C 15.551 24.107 1.00 82.50 С ATOM 794 LYS C 3 CG 12.921 15.895 23.122 1.00 81.54 C ATOM 795 CD LYS C 3 11.926 14.746 23:005 1.00 81.93 C ATOM 796 CE LYS C 3 15.022 10.866 21.952 1.00 80.79 C 797 ATOM NZ LYS C 3 10.154 14.177 16.300 22.214 1.00 82.56 С 798 ATOM C LYS C 3 17.809 25.128 1.00 82.12 C 799 0 ATOM LYS C 3 18.925 17.474 14.053 24.617 1.00 81.76 C ATOM 800 N GLN C 4 13.651 26.302 1.00 80.32 С ATOM 801 CA GLN C 4 12.856 18.401 17.759 27.094 1.00 78.87 c ATOM 802 CB GLN C 4 12.504 28.440 1.00 С 79.91 ATOM 803 CG GLN C 4 12.122 16.275 28.356 1.00 80.66 С ATOM 804 CD GLN C 4 11.087 15.971 27.280 1.00 81.02 C ATOM 805 OE1 4 11.348 9.907 GLN C 1.00 79.52 C 16.140 26.082 ATOM 806 NE2 GLN C 4 15.516 27.701 1.00 81.57 ATOM 807 GLN C C 4 13.667 1.00 77.97 19.680 27.299 C ATOM 808 0 GLN С 4 13.186 20.781 27.032 1.00 78.45 5 ATOM 809 N ILE C 14.902 19.530 27.772 1.00 76.07 C 5 ATOM ILE C 810 CA 15.785 20.670 27.974 1.00 73.89 C ATOM CB 5 811 ILE C 17.206 1.00 73.07 20.220 28.381 ċ 5 ATOM 812 CG2 ILE C 18.175 21.388 28.264 1.00 71.17 000 ATOM ILE C 813 CG1 17.174 19.623 29.795 1.00 72.84 ATOM 814 CD1 ILE C 5 18.518 19.113 30.285 1.00 71.39 5 .5 ATOM 815 С IĻE C 15.880 21.423 26.656 1.00 74.14 O ATOM 816 0 ILE C 15.939 22.651 26.628 1.00 73.70 ATOM N 317 GLU C 6 15.895 20.664 25.567 1.00 73.88 0 ATOM 818 CA GLU C б 15.972 21.222 24.225 1.00 73.70 ATOM GLU C 819 CB 6 16.395 20.135 23.229 72.24 1.00 АТОМ GLU C 820 CG 6 17.787 19.535 23.464 1.00 69.96 С ATOM 821 GLU C CD 6 18.922 20.428 22.985 1.00 68.01 C ATOM 822 OE1 GLU С б 19.044 21.575 23.461 1.00 65.93 C OE2 GLU C ATOM 823 19.702 19.963 22.125 1.00 68.18 С ATOM 824 C GLU C б 14.602 21.773 23.842 1.00 74.50 С ATOM 825 0 GLU C 14.476 22.546 22.890 1.00 75.27 C ATOM 826 N ASP C 13.577 21.372 24.587 1.00 74.82 С ATOM 827 CA ASP C 7 12.218 21.838 24.327 1.00 76.17 C ATOM 828 CB ASP C 11.195 20.742 24.544 1.00 77.40 С MOTA 829 CG ASP C 7 11.408 19.488 23.818 1.00 78.45 C ATOM 930 OD1 ASP C 7 22.580 11.518 19.609 1.00 79.26 C ATOM OD2 ASP C 24.404 11.452 18.380 1.00 79.10 C

Figure 11N

Inventors:

ATOM	832	C	ASF	· c	7	11.90	6 23.079	9 25.160	1.00 7	5 92	С
ATOM	833	0	ASP		7	11.379					C
MOTA	834	N	LYS	C	8	12.223	3 23.024				Č
MOTA	835	CA	LYS	C	8	11.987	7 24.157			1.19	c
ATOM	836	CB	LYS	C	8	12.565				2.69	c
ATOM	837	CG	LYS	C	8	11.647	7 24.225			2.96	č
ATOM	838		LYS	C	8	10.428	3 23.312			5.00	č
ATOM	839		LYS		8	9.587	7 23.471	31.197			c
ATOM	840		LYS		8	8.998	24.829	31.389		3.68	Ċ
ATOM	841	С	LYS		8	12.727	25.319	26.679	1.00 6	9.24	С
ATOM	842		LYS		8	12.295		26.745	1.00 6	9.77	C
ATOM	843	N	ILE		9	13.855		26.046	1.00 6	5.63	С
MOTA	844	CA	ILE		9	14.609		25.362	1.00 64	1.27	С
ATOM	845	CB	ILE		9	15.950			1.00 62	2.88	C
MOTA	846	CG			9	16.585			1.00 62	2.42	C
ATOM	847	CG:			9	16.900			1.00 64	1.19	C
ATOM	848	CD1			9	18.244			1.00 64	1.32	С
ATOM	849	C			9	13.756				.69	С
ATOM ATOM	850 851	0	ILE		9	13.735				3.21	C
ATOM	852	N CA	GLU		10	13.036		23.543		.89	C
ATOM	853	CB	GLU		10 10	12.163	26.092	22.429		.21	C
ATOM	854	CG	GLU		10	11.419	24.865	21.886		.68	C
ATOM	855	CD	GLU		10	10.451 9.688	25.180	20.751		.12	C
ATOM	856	OE1			10	8.874	23.961	20.251		.29	C
ATOM	857	OE2			10	9.894	24.125	19.318		.26	C
ATOM	858	C	GLU		10	11.142	22.845 27.147	20.780		.71	С
ATOM	859	0	GLU		10	10.991	28.157	22.831 22.147		. 65	C
ATOM	860	N		C	11	10.429	26.898	23.927		.16	C
ATOM	861	CA	GLU		11	9.415	27.826	24.435		.41 .98	C
ATOM	862	CB	GLU		11	8.736	27.243	25.683	1.00 58		C
ATOM	863	CG	GLU		11	9.709	26.588	26.652	1.00 61		C
ATOM	864	CD	GLU	С	11	9.376	26.801	28.127	1.00 63		c
ATOM	865	OE1	GLU	С	11	9.329	27.972	28.563	1.00 64		C
ATOM	866	OE2	GLU	C	11	9.184	25.804	28.855		.50	, C
ATOM	867	C	GLU	С	11	10.021	29.186	24.772	1.00 58		C
MOTA	868	0	GLU	С	11	9.519	30.229	24.351	1.00 59		Ċ
ATOM	869	N	ILE		12	11.103	29.178	.25.532	1.00 56	.15	C
ATOM	870	CA		С	12	11.765	30.415	25.902	1.00 56	.41	C
ATOM	871	CB		C	12	13.043	30.139	26.710	1.00 55		С
ATOM	872	CG2		C	12	13.791	31.448	26.950	1.00 52	.26	C
ATOM	873	CG1	ILE ·		12	12.680	29.404	28.008	1.00 55.	.06	C
ATOM	874	CD1	ILE		12	13.858	29.085	28.914	1.00 55.	11	C
ATOM	875	С		C	12	12.132	31.239	24.671	1.00 57.		C
ATOM	876	0	ILE (12	11.944	32.454	24.659	1.00 59.		C
ATOM ATOM	877	N	GLU (13	12.668	30.589	23.642	1.00 60.		C
ATOM	878 879	CA CB	GLU (13	13.039	31.312	22.423	1.00 62.		C
ATOM	880	CG	GLU (13	13.916	30.449	21.497	1.00 66.		C
ATOM	881	CD	GLU (13 13	13.319	29.091	21.138	1.00 70.		С
ATOM	882		GLU (13	14.091	28.355	20.041	1.00 73.		С
ATOM	883		GLU (13	15.330	28.233	20.163	1.00 72.		C
ATOM	884	C	GLU (13	13.456 11.785	27.887	19.064	1.00 73.		C
ATOM	885	0.	GLU (13	11.785	31.748	21.679	1.00 60.		C
ATOM	886	N.	SER C		14	10.695	32.733 31.010	20.946	1.00 61.		C
ATOM	887	CA	SER C		14	9.432	31.010	21.864	1.00 59.		С
ATOM	888	CB	SER C		14	8.392	30.248	21.211 21.439	1.00 60.		C
ATOM	889	OG	SER C		14	7.157	30.248	20.820	1.00 59. 1.00 56.		C
ATOM	890	С	SER C		14	8.921	32.568	20.320	1.00 55.		C
ATOM	891	ō	SER C		14	8.793	33.655	21.730	1.00 51.		c
								, , ,	2.00 39.	50	L

Figure 110

Docket/App No.: 0399.1192-008 Title: Inhibitors of HIV Membrane Fusion

ventors: Debra M. Eckert, et al.

ATOM	892	N	LYS C	15	8.532	32.671	23.091	1.00 62.79	С
ATOM	893	CA	LYS C	15	8.153	33.873	23.771	1.00 64.30	С
ATOM	894	CB	LYS C	15	7.949	33.612	25.273	1.00 65.74	C
	895	CG	LYS C	15	6.637	32.903	25.642	1.00 68.25	C
ATOM		CD	LYS C	15	6.534	32.695	27.154	1.00 69.92	¢
ATOM	896		LYS C	15	5.186	32.131	27.564	1.00 70.69	С
ATOM	897	CE			4.078	33.079	27.241	1.00 73.69	С
MOTA	898	NZ	LYS C	15	9.130	35.029	23.601	1.00 64.03	Ċ
MOTA	899	С	LYS C	15			23.408	1.00 64.04	Ċ
ATOM	900	0	LYS C	15	8.723	36.175	23.408	1.00 63.47	c
ATOM	901	N	GLN C	16	10.418	34.721			C
MOTA	902	CA	GLN C	16	11.451	35.733	23.537	1.00 65.82	C
ATOM '	903	CB	GLN C	16	12.813	35.064	23.393	1.00 65.17	
ATOM	904	CG	GLN C	16	13.970	36.027	23.413	1.00 65.29	C
ATOM	905	CD	GLN C	16	14.944	35.695	24.516	1.00 66.93	C
ATOM	906	OE1	GLN C	16	15.940	36.389	24.719	1.00 68.97	C
ATOM	907	NE2	GLN C	16	14.657	34.621	25.244	1.00 66.55	С
ATOM	908	С	GLN C	16	11.157	36.605	22.317	1.00 67.53	С
ATOM	909	ō	GLN C	16	11.172	37.836	22.397	1.00 68.90	C
ATOM	910	N	LYS C	17	10.886	35.952	21.193	1.00 67.63	C
	911	CA	LYS C	17	10.566	36.648	19.954	1.00 67.83	C
ATOM		CB	LYS C	17	10.355	35.627	18.833	1.00 69.39	С
ATOM	912			17	9.747	36.199	17.556	1.00 72.05	С
ATOM	913	CG			10.657	37.203	16.835	1.00 73.47	С
ATOM	914	CD	LYS C	17	9.946	37.784	15.613	1.00 74.71	Ċ
ATOM	915	CE	LYS C	17			14.795	1.00 76.15	Č
MOTA	916	NZ	LYS C	17	10.885	38.603	20.123	1.00 66.64	Ċ
ATOM	917	С	LYS C	17	9.306	37.492		1.00 67.45	· č
ATOM	918	0	LYS C	17	9.244	38.632	19.652		
ATOM	919	N	LYS C	18	8.300	36.924	20.784	1.00 64.29	C
ATOM	920	CA	LYS C	18	7.049	37.641	21.019	1.00 63.62	C
ATOM	921	CB	LYS C	18	5.979	36.719	21.627	1.00 64.15	
ATOM	922	CG	LYS C	18	5.088	36.062	20.586	1.00 66.52	C
ATOM	923	CD	LYS C	18	3.935	35.297	21.220	1.00 68.98	C
MOTA	924	CE	LYS C	18	4.427	34.076	21.970	1.00 70.96	С
ATOM	925	NZ	LYS C	18	5.098	33.116	21.040	1.00 72.62	C
ATOM	926	C	LYS C	1.8	7.265	38.852	21.922	1.00 61.00	C
ATOM	927	ō	LYS C	18	6.854	39.958	21.585	1.00 61.84	C
ATOM	928	N	ILE C	19	7.904	38.653	23.067	1.00 56.58	С
ATOM	. 929	CA	ILE C	19	8.179	39.765	23.961	1.00 53.92	С
ATOM	930	CB	ILE C	19	9.101	39.329	25.119	1.00 52.10	С
ATOM	931	CG2		19	9.719	40.545	25.799	1.00 51.95	C
	932	CG1		19	8.304	38.463	26.095	1.00 51.65	С
ATOM		CD1		19	9.103	37.908	27.247	1.00 50.93	С
MOTA	933		ILE C	19	8.833	40.893	23.165	1.00 53.24	С
MOTA	934	С	ILE C	19	8.604	42.069	23.438	1.00 52.35	С
ATOM	935	0			9.642	40.534	22.173	1.00 53.82	С
ATOM	936	N	GLU C		10.294	41.536	21.338	1.00.54.86	С
ATOM	937	CA	GLU C	20	11.393		20.472	1.00 55.74	Ċ
ATOM	938	CB	GLU C	20	12.554	40.318	21.251	1.00 56.50	Č
ATOM	939	CG	GLU C			39.851	20.352	1.00 56.98	Č
MOTA	940	CD	GLU C		13.683		19.543	1.00 56.87	Č
MOTA	941	OE1			13.473	38.918		1.00 58.79	C
ATOM	942	OE2			14.786		20.453		C
MOTA	943	C	GLU C		9.245		20.437	1.00 55.80	
ATOM	944	0	GLU C	20	9.311		20.166	1.00 55.44	C
ATOM	945	N	ASN C	21	8.289		19.972	1.00 55.46	C
ATOM	946	CA	ASN C	21	7.223		19.118	1.00 57.62	C
ATOM	947	CB	ASN C		6.392	40.754	18.530	1.00 59.92	C
ATOM	948	ÇG	ASN C		7.060	40.101	17.325	1.00 63.29	C
ATOM	949		ASN C		6.574	39.092	16.806	1.00 62.67	С
ATOM	950	ND:			8.169	40.684	16.866	1.00 61.87	С
ATOM	951	C	ASN C		6.307	42.829	19.891	1.00 58.25	C
ri Ori		-							

Figure 11P

1.00 59.75 43.697 19.309 5.649 952 ASN C 0 ATOM 1.00 56.32 42.645 21.206 6.255 GLU C 953 N ATOM 1.00 53.64 43.489 22.030 22 22 22 5.411 GLU C CA MOTA 954 1.00 55.42 5.014 42.756 23.313 GLU C CB 955 ATOM 1.00 60.12 3.786 43.357 23.967 GLU C CG ATOM 956 Ċ 23.188 1.00 61.82 43.082 2,506 GLU C 22 957 CD MOTA Ċ 43.024 21.942 1.00 62.49 2.559 OE1 GLU C 22 958 C MOTA 23.825 1.00 63.39 42.954 1.435 OE2 GLU C 22 959 ATOM 6.158 22.344 1.00 50.89 44.791 GLU C C 960 ATOM 000000000 5.573 22.282 1.00 49.72 45.873 GLU C 22 0 961 ATOM 22.665 1.00 47.08 7.448 44.691 ILE C 23 N ATOM 962 22.948 1.00 46.40 45.876 8.259 ILE C 23 ATOM 963 CA 9.752 10.707 45.504 23.290 1.00 47.53 ILE C СВ 964 ATOM 1.00 44.86 46.653 22.910 CG2 ILE C MOTA 965 24.783 1.00 45.28 9.898 45.178 CG1 ILE C 23 966 MOTA 44.004 25.256 1.00 45.91 CD1 ILE C 23 9.101 ATOM 967 46.771 21.717 1.00 46.76 ILE C 8.222 C ATOM 968 1.00 46.87 21.822 8.317 ILE C 23 0 C ATOM 969 46.137 20.556 1.00 47.50 ALA C 24 8.071 N 970 MOTA 19.271 1.00 46.10 46.828 CA ALA C 8.002 24 971 MOTA C 45.809 47.644 1.00 44.51 18.126 8.112 ALA C 24 ATOM 972 CB 19.137 1.00 45.09 ALA C 6.706 24 С 973 ATOM 18.752 1.00 43.05 С 48.810 6.741 ALA C 24 ATOM 974 О 1.00 43.64 C 19.445 47.034 47.753 ARG C 25 5.566 975 N MCTA 19.346 1.00 45.79 С ARG C 25 4.301 CA 976 ATOM 1.00 44.07 С ARG C 19.581 3.115 46.807 25 977 CB ATOM С 18.564 1.00 48.16 ARG C 3.045 45.680 25 MOTA 978 CG С 1.00 50.13 18.458 ARG C. 1.677 44.986 25 ATOM 979 CD C 19.564 1.00 1.216 44.299 ARG C 25 980 ΝE MOTA 20.725 1.00 58.36 С 0.665 44.888 ARG C 25 981 CZ ATOM 1.00 59.26 C 0.475 46.206 20.756 25 NH1 ARG C 982 MOTA 21.755 1.00 59.83 ¢ 0.268 44.148 NH2 ARG C 25 ATOM 983 C 1.00 47.24 ARG C 4.257 20.345 25 48.908 984 С MOTA 19.978 1.00 50.68 С 3.941 50.038 25 985 0 ATOM С 21.601 1.00 47.54 ILE C 4.584 48.617 26 986 N ATOM С 1.00 44.40 ILE C 49.608 22.673 4.591 26 987 CA ATOM С 1.00 43.91 24.001 48.959 5.042 26 MOTA 988 CB 1.00 45.47 5.259 50.026 25.071 CG2 ILE C 26 989 ATOM 24.450 1.00 42.59 4.010 47.930 CG1 ILE C 26 990 ATOM 1.00 40.19 4.445 47.138 25.663 CD1 ILE C 26 991 ATOM 1.00 44.58 C 22.379 50.766 5.532 26 992 C ILE C ATOM 1.00 42.04 ILE C 26 5.193 51.935 22.564 993 ATOM С 1.00 46.75 21.919 27 27 27 6.721 50.422 N АТОМ 994 1.00 51.78 LYS C 51.394 21.619 7.754 995 ATOM CA C 8.915 50.674 20.951 1.00 54.23 996 CB ATOM С 1.00 57.21 LYS C 27 27 51.465 20.863 10.184 997 ÇG ATOM 1.00 60.99 11.313 50.479 20.644 998 ÇD ATOM 1.00 62.83 51.064 21.014 12.660 999 CE LYS C 27 ATOM 1.00 64.49 13.750 50.060 20.828 27 NZ LYS C 1000 ATOM 1.00 52.44 52.556 20.750 7.299 LYS C 27 1001 С ATOM C 7.334 53.710 21.165 1.00 54.11 LYS C 27 0 1002 ATOM C 6.877 52.239 19.538 1.00 53.88 LYS C 28 1003 MOTA C 53.250 18.599 1.00 55.29 6.435 LYS C 28 CA 1004 MOTA C 17.249 1.00 57.59 6.169 7.390 52.582 CB LYS C 28 1005 ATOM Ċ 16.717 1.00 59.15 51.841 CG LYS C 28 1006 MOTA С 15.635 1.00 62.19 50.830 28 7.041 LYS C 1007 CD MOTA 15.158 1.00 63.12 50.088 8.292 CE LYS C 28 1008 MOTA 49.411 16.282 1.00 65.69 TAR C 9.029 28 NZ 1009 ATOM 19.122 1.00 55.14 5.187 53.931 28 1010 MOTA C

Figure 11Q

19.030

1.00

55.147

5.052

LYS

ATOM

1011

ATOM

1012 N

Docket/App No.: 0399.1192-008

29

Title: Inhibitors of HIV Membrane Fusion Debra M. Eckert, et al. Inventors:

LEU C 4.275 53.138 19.671 1.00 52.27 ATOM 1013 CA LEU C 29 3.025 53.649 20.214 1.00 51.04 ATOM 1014 CB LEU C 29 2.281 52.485 20.855 1.00 51.13 MOTA 1015 CG LEU C 29 0.776 52.493 21.051 1.00 50.66 ATOM 1016 CD1 LEU C 29 52.868 0.051 19.755 1.00 51.59 ATOM 1017 CD2 LEU C 29 0.389 51.100 21.491 1.00 50.29 ATOM 1018 C LEU C 29 3.347 54.739 21.245 1.00 50.83 ATOM 1019 0 LEU C 29 2,739 4.327 55.805 21.269 1.00 53.58 ATOM 1020 N LEU C 54.457 22.089 1.00 50.52 ATOM 1021 CA LEU C 30 4.767 55.397 23.100 1.00 48.88 ATOM 1022 CBLEU C 30 5.813 54.730 23.997 1.00 48.03 ATOM 1023 CG LEU C 30 6.485 55.530 25.113 1.00 47.31 ATOM 1024 CD1 LEU C 30 5.447 56.172 26.033 1.00 45.24 ATOM 1025 CD2 LEU C 30 7.398 54.575 25.889 1.00 48.28 ATOM 1026 С LEU C 30 5.374 56.587 22.379 1.00 48.83 ATOM 1027 0 LEU C 30 5.020 1.00 48.40 57.736 22.642 ATOM 1028 N GLN C 31 6.298 56.289 21.470 1.00 49.93 ATOM 1029 CA GLN C 31 20.670 6.983 57.304 1.00 52.00 GLN C ATOM 1030 CB 31 7.822 56.609 19.590 1.00 55.56 ATOM 1031 CG GLN C 31 8.628 57.513 18.645 1.00 61.26 ATOM 1032 CD GLN C 31 9.768 58.241 19.333 1.00 64.58 ATOM 1033 OE1 GLN C 31 10.233 57.818 20.391 1.00 68.00 ATOM 1034 NE2 GLN C 31 10.249 59.318 18.715 1.00 64.37 ATOM 1035 GLN C 31 5.947 58.225 20.009 1.00 49.56 ATOM 1036 GLN C 31 6.192 59.415 19.814 1.00 45.68 C ATOM 1037 N LEU C 32 4.793 57.657 19.675 1.00 47.64 C ATOM 1038 CA LEU C 32 3.723 58.401 19.034 1.00 48.95 С ATOM 1039 CB LEU C 32 2.689 57.433 18.461 1.00 50.72 00000 ATOM 1040 CG LEU C 32 1.602 57.935 17.502 1.00 51.93 ATOM 1041 CD1 LEU Ç 32 2.209 58.293 16.154 1.00 50.26 ATOM 1042 CD2 LEU C 32 0.554 56.840 17.313 1.00 51.55 ATOM 1043 С LEU C .32 3.070 59.295 20.077 1.00 49.32 ATOM 1044 0 LEU C 32 3.040 60.519 19.929 1.00 50.01 С ATOM 1045 N THR C 33 2.545 58.659 21,125 0 1.00 48.74 ATOM 1046 CA THIR C 33 1.878 59.324 22.246 1.00 43.86 MOTA 1047 CB THR C 33 1.643 58.329 23.400 C 1.00 46.04 ATOM 1048 OG1 THR C 33 0.707 57.332 22.977 1.00 47.18 ATOM 1049 CG2 THR C 33 1.121 24.639 22.771 59.039 1.00 42.89 000 ATOM 1050 THR C С 33 2.683 60.494 1.00 41.04 MOTA 1051 0 THR C 33 2.132 61.537 23.122 1.00 39.26 ATOM 1052 Ν VAL C 3.992 34 60.303 1.00 38.83 22.843 c ATOM 1053 CA VAL C 34 4.886 61.346 23.301 С ATOM 1054 VAL C CB 34 6.329 60.825 23.377 1.00 33.71 ATOM 1055 CG1 34 7.270 23.904 61.907 CG1 VAL C
CG2 VAL C
C VAL C
O VAL C
N TRP C
CA TRP C
CB TRP C 1.00 29.40 ATOM 1056 34 6.366 59.590 24.251 1.00 31.78 ATOM 1057 34 4.795 62.437 22.254 1.00 38.65 С ATOM 1058 34 4.489 63.595 22.556 1.00 39.38 C ATOM 1059 35 5.049 62.038 21.010 1.00 42.18 ATOM 1060 35 5.002 62.937 19.868 1.00 40.00 C ATOM 1061 35 4.991 62.134 18.563 1.00 40.06 ATOM 1062 CG TRP C 35 4.848 63.020 1.00 36.56 17.399 С ATOM CD2 TRP C 1063 63.161 35 3.696 16.561 1.00 36.91 ATOM 1064 CE2 TRP C 35 3.968 64.212 15.673 1.00 41.20 ATOM 1065 CE3 TRP C 35 2.457 62.505 16.503 1.00 40.31 ATOM 1066 CD1 TRP C 35 5.748 63.944 16.974 1.00 35.30 С ATOM 1067 NE1 TRP C 5.228 64.673 15.945 1.00 39.45 C ATOM 1068 CZ2 TRP C 35 3.037 64.643 14.704 1.00 38.75 C ATOM 1069 CZ3 TRP C 35 1.528 62.934 15.541 1.00 39.54 С 1070 ATOM CH2 TRP C 35 1.827 63.984 14.651 1.00 41.30 ATOM Ç 2073 С TRP C 3.764 1.00 39.80 63.833 19.901

С

Figure 11R

ATOM	1072	0	TRP	С	35	3.86		65.052	19.769	1.00 38.3		
ATOM	1073	N	GLY	С	36	2.60		63.210	20.059	1.00 36.8		
ATOM	1074	CA		С	36	1.35		63.957	20.103	1.00 38.9		
MOTA	1075	С		C	36	1.33		64.973	21.226	1.00 38.4		
ATOM	1076	0		С	36	0.93		66.114	21.001	1.00 37.7		
MOTA	1077	N		C	37	1.70		64.557	22.435	1.00 36.0		
ATOM	1078	CA		C	37	1.7		65.442	24.857	1.00 36.0		
ATOM	1079	CB		C	37	2.33		64.755 65.766	26.005	1.00 27.3		
ATOM	1080	CG2		C	37	2.48 1.5	3 '	63.548	25.275	1.00 37.3		
ATOM	1081	CG1		C	37 37	2.0		62.794	26.501	1.00 35.		
ATOM	1082	CD1		C	37	2.5		66.655	23.284	1.00 38.		
MOTA	1083	C		C	37	2.1		67.788	23.529	1.00 37.	68 C	
ATOM	1084	O N		C	38	3.7		66.399	22.740	1.00 40.3		
MOTA	1085 1086	CA	LYS		38	4.7		67.456	22.381	1.00 42.		
MOTA	1087	CB	LYS	c	38	5.9		66.868	21.639	1.00 46.		
MOTA MOTA	1088	CG		Č	38	7.1		67.829	21.391	1.00 52.		
ATOM	1089	CD		c	38	8.1	25	67.162	20.433	1.00 56.		
ATOM	1090	CE		Ċ.	38	9.3	65	68.008	20.096	1.00 56.		
ATOM	1091	NZ		C	38	10.3	40	68.155	21.222	1.00 59.		
ATOM	1092	C	LYS	С	38	3.9	95	68.445	21.483	1.00 42.		
ATOM	1093	0	LYS	С	38	4.3	51	69.628	21.428	1.00 41.		
ATOM	1094	N	GLN	C	39	2.9		67.966	20.774	1.00 39.		
MOTA	1095	CA	GLN	С	39	2.2		68.862	19.908	1.00 40.		
ATOM	1096	CB		С	39	1.4		68.100	18.778	1.00 41.		
ATOM	1097	CG	GLN		39	2.3		67.148	17.928 17.465	1.00 42.		
ATOM	1098	CD		C	39	3.6		67.786	16.813	1.00 44.		
MOTA	1099	OE1			39	3.6		68.822 67.163	17.802	1.00 46.		
MOTA	1100	NE2			39	4.8 1.2		69.638	20.781	1.00 36.		
MOTA	1101.	Ç .	GLN		39 39	1.3		70.845	20.885	1.00 34.		
ATOM	1102	0	GLN LEU		40	0.2		68.950	21.398	1.00 34.		
ATOM	1103	N CA	LEU		40	-0.6		69.625	22.268	1.00 36.		
MOTA	1104 1105	CB	LEU		40	-1.4		68.595	23.096	1.00 34.		
ATOM ATOM	1105	CG	LEU		40	-2.3		69.192	24.186	1.00 34.		
ATOM	1107		LEU		40	-3.3		70.142	23.510	1.00 34.		
ATOM	1108		LEU		40	-3.0	57	68.084	24.972	1.00 30.		
ATOM	1109	C	LEU		40	-0.0	29	70.630	23.226	1.00 36.		
ATOM	1110	Ō	LEU		40	-0.4	94	71.755	23.419	1.00 36.		
ATOM	1111	N	GLN	С	41	1.0		70.220	23.832	1.00 36.		
ATOM	1112	CA	GLN	С	41	1.7		71.106	24.751	1.00 38.		
ATOM	1113	CB	GLN	С	41	2.8		70.310	25.433	1.00 38.		
MOTA	1114	CG	GLN		41	3.6		70.994	26.582 27.529	1.00 40.		
ATOM	1115	CD	GLN		41	4.2		69.979 69.028	27.091	1.00 53.		
MOTA	1116		GLN		41	4.8		70.180	28.831	1.00 52.		
MOTA	1117	NE2			41	4.0		72.336	23.998	1.00 37.		
ATOM	1118	C	GLN		41	2.1		73.466	24.486	1.00 38.		
MOTA	1119	0	GLN		41	2.8		72.128	22.795	1.00 36.	75 C	
MOTA	1120	N CA	ALA ALA		42	3.3		73.249	22.014	1.00 36.	93 C	
MOTA	1121	CB	ALA		42	4.0		72.717	20.779	1.00 32.		
MOTA	1123	C	ALA		42	2.2		74.209	21.600	1.00 35.		
MOTA MOTA	1124	ō	ALA		42	2.4		75.427	21.602	1.00 34.		
ATOM	1125	N	ARG		43	1.1		73.629	21.249	1.00 32.		
ATOM	1126	CA	ARG		43	-0.0		74.365	20.829	1.00 34.		
MOTA	1127	CB	ARG		43	-1.1	152	73.357	20.524	1.00 34.		
MOTA	1128	CG	ARG		43	-2.4		73.891	20.060	1.00 36.		
ATOM	1129	CD	ARG	C	43	-3.3		72.667	19.769	1.00 37.		
ATOM	1130	NE	ARG		43	-4.6		72.945	19.236	1.00 40.		
ATOM	1131	CZ	ARG	C	43	-5.4	481	71.985	18.901	1.00 42.	. / =	

Figure 11S

Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion Leventors: Debra M. Eckert, et al.

```
1.00 41.40
                                          70.717
                                                   19.051
                                  -5.127
             NH1 ARG C
NH2 ARG C
C ARG C
                         43
MOTA
       1132
                                                                             С
                                                            1.00 44.00
                                                   18.421
                                           72.288
                                  -6.676
                         43
                                                                             000
ATOM
       1133
                                                            1.00 37.96
                                                   21.883
                                  -0.568
                                           75.347
                         43
       1134
MOTA
                                                            1.00 36.78
                                                   21.558
                                           76.425
                                  -1.049
                  ARG C
       1135
                         43
                                                            1.00 41.66
ATOM
                                           74.971
                                                   23.151
                                  -0.434
                  ILE C
                         44
       1136
                                                                              C
MOTA
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                                           75.799
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                  ILE C
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       1137
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ATOM
                                                            1.00 46.21
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                                           75.717
                                  -1.802
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                  ILE C
       1139
              CG2
MOTA
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                                                   24.876
                  ILE C
                                  -2.572
                                           74.041
                          44
              CG1
       1140
                                                            1.00 50.31
ATOM
                                                   25.786
                                  -2.926
                                           72.877
                          44
              CD1
       1141
ATOM
                                                            1.00 41.15
                                           76.802
                                                   24.807
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                  ILE C
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       1142
                                                                              C
MOTA
                                                            1.00 40.03
                                           77.961
                                                    25.047
                                   -0.235
                          44
                  ILE C
MOTA
       1143
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                                                            1.00 40.33
                                                    25.005
                                           76.350
                                   1.345
              N
                  LEU C
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       1144
ATOM
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                                                            1.00 39.81
                                           77.184
                                                    25.579
                                    2.401
                  LEU C
                          45
              CA
       1145
                                                            1.00 40.22
ATOM
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                                                                              C
                                           76.322
                                    3.357
              CB
                  LEU C
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                                                            1.00 40.80
                                           75.608
                                                    27.694
                                    2.889
                  LEU C
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              CG
MOTA
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                                                            1.00 42.51
                                           74.714
                                                    27.364
                                    1.733
                  LEU C
                          45
              CD1
MOTA
        1148
                                                            1.00 39.44
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                                           74.789
                                                    28.299
                                    4.029
              CD2 LEU C
                          45
        1149
                                                            1.00 38.95
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MOTA
                                           77.953
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                                    3.215
                          45
              C
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ATOM
        1150
                                                             1.00 39.83
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                                           77.689
                                                    23.327
                                    3.071
                   LEU C
                          45
              0
MOTA
        1151
                                                             1.00 39.47
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                                                    24.964
                                            78.810
                                    4.014
              NT
                  LEU C
ATOM
        1152
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                                                             1.00 38.82
                                                    27.138
                                           62,369
              OH2 TIP W
                           2
                                    8.280
        1153
                                                             1.00 78.47
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MOTA
                                           24.001
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                                   28.782
              OH2 TIP W
ATOM
        1154
                                                             1.00 50.43
                                                                              W
                                            62.209
                                                    33.896
                                    0.492
              OH2 TIP W
ATOM
        1155
                                                             1.00 45.29
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                                                    23.199
                                    6.020
                                            70.609
                            5
              OH2 TIP W
        1156
                                                             1.00 37.25
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 ATOM
                                                    31.896
                                            78.695
               OH2 TIP W
                                    1.993
        1157
 ATOM
                                                             1.00 49.56
                                            18.975
                                                    19.485
                                   20.294
               OH2 TIP W
        1158
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 ATOM
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                                            15.442
                                                    35.405
                                   18.592
               OH2 TIP W
        1159
 ATOM
                                                             1.00 31.24
                                                    32.524
                                            64.337
               OH2 TIP W
                                   -5.907
        1160
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 ATOM
                                                    30.945
                                                             1.00 47.94
                                            18.853
               OH2 TIP W
                           10
                                   11.567
        1161
 ATOM
                                                    23.794
                                                             1.00 46.60
                                            65.456
               OH2 TIP W
                                    -9.321
                           11
        1162
 MOTA
                                                             1.00 59.15
                                            65.953
                                                    28.078
                                   -2.842
               OH2 TIP W
                           1.2
 MOTA
        1163
                                                                  37.51
                                                    18.859
                                                             1.00
                                            77.305
                                    -1.409
               OH2 TIP W
                           13
 ATOM
        1164
                                                             1.00 39.02
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                                    -5.597
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        1165
 MOTA
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                                            75.908
               OH2 TIP W
                                    -5.079
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        1166
 ATOM
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                                            58.431
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                                   12.444
               OH2 TIP W
                           16
        1167
 ATOM
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                                            70.555
                                                     24.520
                                   -12.927
               OH2 TIP W
                           17
        1168
 ATOM
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                                            23.356
                                   14.897
               OH2 TIP W
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         1169
 ATOM
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                                            40.721
                                                     28.964
                                    3.154
               OH2 TIP W
                           19
 ATOM
         1170
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                                     4.290
                                            81.951
                           20
               OH2 TIP W
         1171
 ATOM
                                                     32.265
                                                             1.00 62.67
                                    26.490
                                            23.104
                           21
               OH2 TIP W
 ATOM
         1172
                                                             1.00 54.53
                                                     33.622
                                            59.162
                                    13.085
                           22
               OH2 TIP W
         1173
 ATOM
                                                              1.00 56.34
                                            45.626
                                                     35.200
                                    -0.166
                           23
               OH2 TIP W
         1174
                                                             1.00 64.05
 мота
                                                     33.867
                                   -10.278
                                            62.692
         1175
                OH2 TIP W
                           24
 ATOM
                                                     29.710
                                                              1.00100.00
                                            10.892
                                    22.697
                           25
                OH2 TIP W
         1176
                                                                               W
 ATOM
                                                     26.136
                                                              1.00 62.29
                                     4.281
                                            39.194
         1177
                OH2 TIP W
                           26
                                                                               W
 ATOM
                                                              1.00 59.57
                                                     19.882
                                    22.833
                                            20.843
                           27
                OH2
                   TIP W
         1178
  ATOM
                                                              1.00 53.18
                                                                               W
                                                     23.517
                                   -10.030
                                             74.838
                           28
         1179
                OH2 TIP W
 ATOM
                                                              1.00 36.18
                                                     24.973
                                    1.246
                                             80.456
                           29
                OH2
                   TIP W
         1180
                                                                               W
  MOTA
                                                              1.00 50.44
                                                     17.506
                                    -3.034
                                             76.181
                           30
         1181
                OH2 TIP W
                                                              1.00 44.03
  ATOM
                                                     18.155
                                     1.424
                                             49.275
                            31
         1182
                OH2
                    TIP W
                                                                               W
  ATOM
                                                              1.00 31.68
                                                     23.710
                                             64.921
                                     6.269
                OH2 TIP W
                            32
         1183
                                                                               W
  ATOM
                                                              1.00 60.31
                                                     40.798
                                             28.497
                                    27.134
                OH2
                    TIP W
                            33
         1184
                                                              1.00 85.52
  ATOM
                                                     41.517
                                             28.221
                                    24.326
                OH2 TIP W
                            34
         1185
  MOTA
                                                     31.850
                                                              1.00
                                                                   68.20
                                                                               W
                                             26.009
                                    24.492
                OH2 TIP W
                            35
         1186
  ATOM
                                                              1.00
                                                                   45.61
                                                                               W
                                                     41.621
                                    17.270
                                             23.540
                OH2 TIP W
                            36
         1187
  ATOM
                                                     41.299
                                                              1.00
                                    17.175
                                             27.169
                он2
                    TIP W
                            37
         1188
  MOTA
                                                              1.00 94.65
                                                     42.769
                                             30.154
                                     17.133
                OH2 TIP W
                            38
         1189
  ATOM
                                                     38.207
                                                              1.00
                                                                   73.43
                                                                                w
                                             29.473
                                     23.961
                OH2
                    TIP W
                            39
          1190
  ATOM
                                                              1.00 86.46
                                                     35.030
                                             30.299
                                     26.646
                OH2 TIP W
                            40
          1191
  ATOM
```

Figure 11T

Docket/App No.: 0399.1192-008

Title: Inhibitors of HIV Membrane Fusion Investors: Debra M. Eckert, et al.

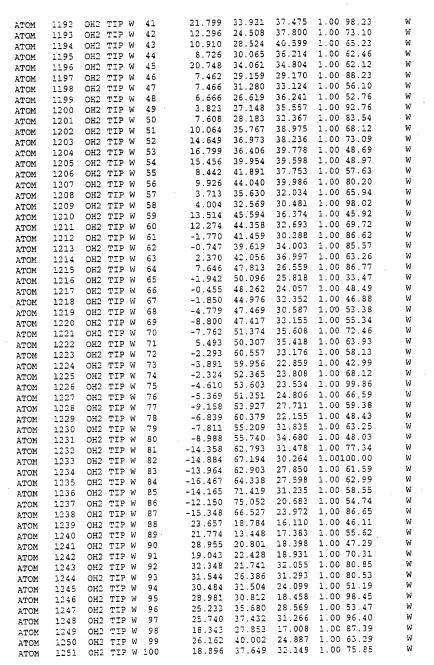


Figure 11U

							W
MOTA	1252	OH2 TIP W 101	20.897	31.301	18.264	1.00 88.40	·W
ATOM	1253	OH2 TIP W 102	19.191	42.582	21.453	1.00 78.30	W
MOTA	1254	OH2 TIP W 103	23.958	41.188	22.932	1.00 54.59	W
MOTA	1255	OH2 TIP W 104	18.433	46.716	25.042	1.00 59.94	W
ATOM	1256	OH2 TIP W 105	22.353	48.547	34.496	1.00 78.60	W
ATOM	1257	OH2 TIP W 106	21.797	41.049	33.535	1.00 75.53	W
ATOM	1258	OH2 TIP W 107	21.437	46.210	21.380	1.00 54.65	W
ATOM	1259	OHE TIP W 108	14.907	43.959	19.119	1.00 58.03	W
ATOM	1260	OH2 TIP W 109	15.635	42.456	33.666	1.00 80.58	W
ATOM	1261	OH2 TIP W 110	19.533	44.310	29.399	1.00 60.97	W
ATOM	1262	OH2 TIP W 111	18.747	50.736	28.680	1.00 55.70	W
MOTA	1263	OH2 TIP W 112	21.131	52.757	38.133	1.00 72.59	W
ATOM	1264	OH2 TIP W.113	17.303	55.311 58.215	28.845	1.00 79.75	W
ATOM	1265	OH2 TIP W 114	18.939	59.680	28.964	1.00 50.64	. W
ATOM	1266	OH2 TIP W 115	14.666	62.649	28.523	1.00 74.43	W
ATOM	1267	OH2 TIP W 116	17.408	61.533	23.810	1.00 89.64	W
MOTA	1268	OH2 TIP W 117	12.106	60.131	37.626	1.00 89.60	W
MOTA	1269	OH2 TIP W 118	10.138	60.131	36.831	1.00 78.03	W
ATOM	1270	OH2 TIP W 119	14.125	65.584	27.400	1.00 63.28	W
MOTA	1271	OH2 TIP W 120	6.987	65.761	30.950	1.00 64.96	W
MOTA	1272	OH2 TIP W 121	8.699	66.582	33.458	1.00 45.24	W
MOTA	1273	OH2 TIP W 122	11.912 7.712	69.520	31.053	1.00 89.81	W
ATOM	1274	OH2 TIP W 123	0.300	66.328	28.053	1.00 83.63	W
MOTA	1275	OH2 TIP W 124	18.739	12.093	36.575	1.00 68.16	W
MOTA	1276	OH2 TIP W 125	8.341	17.901	23.874	1.00 69.12	M
ATOM	1277	OH2 TIP W 126	6.665	20.667	30.766	1.00 79.31	W
ATOM	1278	OH2 TIP W 127	13.178	21.216	32.239	1.00 55.97	W
MOTA	1279	OH2 TIP W 128	7.700	21.187	21.255	1.00 66.56	W
MOTA	1280	OH2 TIP W 129	17.038	26.024	19.828	1.00 40.17	W
ATOM	1281	OH2 TIP W 130	9.682	31.384	16.376	1.00 77.12	W
ATOM	1282	0112 1 1 2 2	11.568	29.117	15.187	1.00 59.43	. W
MOTA	1283		2.602	30.287	27.387	1.00 64.52	W
MOTA	1284		10.743	41.812	16.813	1.00 84.35	W
MOTA	1285	OH2 TIP W 134 OH2 TIP W 135	13.070	38.706	12.664	1.00 61.24	W
MOTA	1286		9.262	44.518	14.939	1.00 51.92	W
ATOM	1287	OH2 TIP W 136 OH2 TIP W 137	12.139	53.137	17.554	1.00 56.22	W
MOTA	1288	OH2 TIP W 138	14.403	57.453	15.838	1.00 66.72	W W
MOTA	1289	OH2 TIP W 139	11.017	71.423	23.035	1.00 71.76	W
ATOM	1290 1291	OH2 TIP W 140	10.451	75.718	24.795	1.00 58.85	W
MOTA	1292	OH2 TIP W 141	11.223	65.048	21.172	1.00 84.46	W
ATOM	1293	OH2 TIP W 142	8.196	70.691	21.387	1.00 66.14	W
ATOM	1294	OH2 TIP W 143	3.381	51.168		1.00 51.91	W
ATOM	1295	OH2 TIP W 144	13.735	48.059		1.00 73.18	W
MOTA	1296	OH2 TIP W 145	2.524	42.027			W
ATOM	1297	OH2 TIP W 146	2.024	39.150			W
MOTA MOTA	1298	OH2 TIP W 147	0.486				W
ATOM	1299	OH2 TIP W 148	0.060				W
	1300	OH2 TIP W 149	14.261		454		W
MOTA MOTA	1301	150					W
ATOM		151					W
ATOM		117	0.421				ï
ATOM		CL-1 CL I 1	13.184	36.734	27.569	1.00 02.04	_
END							
				T:	. 113/		

Figure 11V